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Groundwater Services, Inc.

Houston, Texas

BIOSCREEN - Groundwater Contamination Natural Attenuation Model (Version 1.3)

Developed by Groundwater Services, Inc., Houston, Texas
for the Air Force Center for Environmental Excellence.

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This file contains information which you need to successfully install BIOSCREEN, as well as information which was developed since the help file was generated. For further information, consult the Windows Help file BIOSCRN.HLP.

Contents:

1.0 Before You Start

BIOSCREEN is a software tool to be used to model groundwater plume migration, taking into account the effects of natural attenuation and biodegradation of mobile contaminants. The BIOSCREEN system consists of the following files:

README.WRI (this file)	Background information and installation instructions.
BIOSCRN.XLS	The BIOSCREEN program file, in Microsoft Excel 5.0 format
BIOSCRN.HLP	The online help file, in Windows Help format.
BIOSCRN.PDF	The full documentation, in Adobe PDF format
EXAMPLES.PDF	Case Study information (Appendix A.6) in Adobe PDF format

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1.1 Quick Start

Run SETUP.EXE from the floppy drive, either by selecting Run from the File menu in Program Manager or by double-clicking on the file SETUP.EXE in File Manager (or Windows 95 Explorer). The installation process creates the C:\BIOSCRN subdirectory on your hard drive, unless you install it elsewhere, and copies BIOSCRN.XLS, BIOSCRN.HLP, and this README.WRI file into the new directory

To run BIOSCREEN after installation, start Microsoft Excel and open the BIOSCRN.XLS file. Fill in your field or hypothetical data into the blanks provided and select either the Run Centerline (centerline model) or Run Array (three-dimensional plume migration model) buttons. Loading from

within Excel is preferred to double-clicking the filename in file manager (see Section 3.0 for an explanation of the evils you will avoid). Alternatively, you can add your new BIOSCREEN directory to your path.

1.2   Minimum System Requirements

Any PC-Compatible computer system capable of running Microsoft Excel version 5 0 for Windows will be able to run BIOSCREEN. Because of the intensive floating point calculations used in the model, however, GSI recommends that the following minimum requirements be observed to ensure a minimum standard of performance:

An Intel 486 CPU, operating at 50 MHz or faster
8MB Random Access Memory (16 MB or more will improve performance)
1MB free hard drive space (for BIOSCREEN only - Excel will require substantially more)

1.3   Software Requirements

BIOSCREEN is designed to be run under Microsoft Excel for Windows. Your system must be running Windows 3.1 or Windows for Workgroups 3.11 and have Excel for Windows version 5.0 or later properly installed.

BIOSCREEN has been tested on Excel version 5.0 for Windows on systems running Windows 3.1, Windows for Workgroups 3.11, Windows 95, and Windows NT Version 3.51 and Excel 7.0 on Windows 95 and Windows NT 3.51. Although no substantial problems were seen with any of these configurations, preliminary reports suggest that users of Excel versions prior to the 'c' maintenance release (versions 5.0 and 5.0a) may experience difficulties under some circumstances. We are researching this issue.

2.0   Installation

1. Run SETUP.EXE from the Windows Program Manager by selecting Run from the File Menu and typing A.SETUP, or run it from File Manager by double-clicking its icon This will create the directory BIOSCRN and copy the essential files (listed above) to that directory

2. Start Microsoft Excel and open the BIOSCRN XLS file. Fill in your field or hypothetical data into the blanks provided and select either the Run Centerline (centerline 2D model) or Run Array (three-dimensional plume migration model) buttons. The unshaded (white) cells are intended to receive your data, while light grey cells may contain either your data or a default formula (re-inserted into the cells by clicking the "Restore Default Formulas" button on the main input screen). Dark grey cells contain only formulas used by the BIOSCREEN system, and should not be changed by the user.

3   You can load and view the online Help by double-clicking its filename in the File Manager pane or by selecting the help button from the BIOSCREEN interface

3.0   Troubleshooting

When I try to get online help, the Windows help program starts, but a dialog box tells me it cannot open the help file. Close BIOSCREEN, leaving Excel running. From the File menu, select Open Browse the directory structure until you find BIOSCRN.XLS, and open it. Now, the Help button will open the proper help file. See online help for additional (more permanent) methods of solving this problem.

The Input screen appears, but it is very small or its edges extend off the screen. The system was designed to operate at a resolution of 640x480 pixels, or standard VGA resolution If you are using a higher resolution, you may either change your video driver in Windows Setup to standard VGA resolution or modify the ZoomFactor to account for your configuration See online help for Display configuration information and instructions for changing the ZoomFactor

4 0   Additional Information

4.1 Printing the BIOSCREEN Data Screens

If you want to print the data in your input screen, the centerline model screen, or the 3-D graph screen, a named range for each has been pre-configured. By pressing F5 and selecting the Print_Area range, the screen you are printing will be highlighted. The same range name exists for each screen. Printing any other part of the worksheets will require resetting the print area. Consult the Excel documentation for instructions on how to accomplish this.

4.2 Electronic Manual Availability

The full documentation set for BIOSCREEN is also available in Adobe Portable Document Format (PDF). Two separate files are available, the manual and a set of two sample problems which illustrate a realistic application of BIOSCREEN. Consult the on-line help file (BIOSCRN.HLP) for sources for this electronic documentation. These files duplicate the contents of the printed documentation.

BIOSCREEN

Natural Attenuation
Decision Support System

User's Manual

Version 1.3

JUNE 1996

Distribution is unlimited; approved for public release.

TECHNOLOGY TRANSFER DIVISION
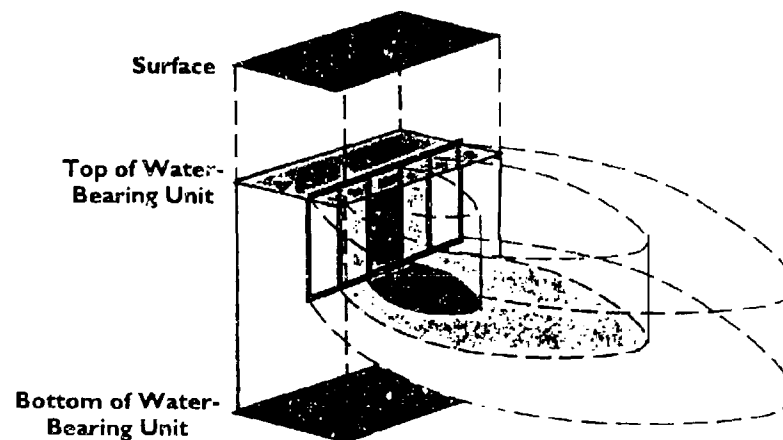
AIR FORCE CENTER FOR ENVIRONMENTAL EXCELLENCE (AFCEE)

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BIOSCREEN

**Natural Attenuation
Decision Support System**

Version 1.3
June 1996

User's Manual

Surface

Top of Water-
Bearing Unit

Bottom of Water-
Bearing Unit

by

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BIOSCREEN Natural Attenuation Decision Support System
Air Force Center for Environmental Excellence Technology Transfer Division

INTRODUCTION

BIOSCREEN is an easy-to-use screening model which simulates remediation through natural attenuation (RNA) of dissolved hydrocarbons at petroleum fuel release sites. The software, programmed in the Microsoft® Excel spreadsheet environment and based on the Domenico analytical solute transport model, has the ability to simulate advection, dispersion, adsorption, and aerobic decay as well as anaerobic reactions that have been shown to be the dominant biodegi dation processes at many petroleum release sites. **BIOSCREEN** includes three different model types:

1) *Solute transport without decay,*

2) *Solute transport with biodegradation modeled as a first-order decay process (simple, lumped-parameter approach),*

3) *Solute transport with biodegradation modeied as an "instantaneous" biodegradation reaction (approach used by BIOPLUME models)*

The model is designed to simulate biodegradation by both aerobic and anaerobic reactions. It was developed for the Air Force Center for Environmental Excellence (AFCEE) Technology Transfer Division at Brooks Air Force Base by Groundwater Services, Inc., Houston, Texas.

INTENDED USES FOR BIOSCREEN

BIOSCREEN attempts to answer two fundamental questions regarding RNA:

1. **How far will the dissolved contaminant plume extend if no engineered controls or further source zone reduction measures are implemented?**

   BIOSCREEN uses an analytical solute transport model with two options for simulating in-situ biodegradation: first-order decay and instantaneous reaction. The model will predict the maximum extent of plume migration, which may then be compared to the distance to potential points of exposure (e.g., drinking water wells, groundwater discharge areas, or property boundaries). Analytical groundwater transport models have seen wide application for this purpose (e.g., ASTM 1995), and experience has shown such models can produce reliable results when site conditions in the plume area are relatively uniform.

2. **How long will the plume persist until natural attenuation processes cause it to dissipate?**

   BIOSCREEN uses a simple mass balance approach based on the mass of dissolvable hydrocarbons in the source zone and the rate of hydrocarbons leaving the source zone to estimate the source zone concentration vs. time. Because an exponential decay in source zone concentration is assumed, the predicted plume lifetimes can be large, usually ranging from 5 to 500 years. Note this is an unverified relationship as there are few data showing source concentrations vs. long time periods, and the results should be considered order-of-magnitude estimates of the time required to dissipate the plume.

BIOSCREEN is intended to be used in two ways:

1. **As a screening model to determine if RNA is feasible at a site.**

   In this case, BIOSCREEN is used early in the remedial investigation to determine if an RNA field program should be implemented to quantify the natural attenuation

occurring at a site. Some data, such as electron acceptor concentrations, may not be available, so typical values are used. In addition, the model can be used to help develop long-term monitoring plans for RNA projects.

2. **As the primary RNA groundwater model at smaller sites.**

The Air Force Intrinsic Remediation Protocol (Wiedemeier, Wilson, *et al.*, 1995) describes how groundwater models may be used to help verify that natural attenuation is occurring and to help predict how far plumes might extend under an RNA scenario. At large, high-effort sites such as Superfund and RCRA sites, a more sophisticated model such as BIOPLUME is probably more appropriate. At less complicated, lower-effort sites such as service stations, BIOSCREEN may be sufficient to complete the RNA study. (Note: "Intrinsic remediation" is a risk-based strategy that relies on RNA).

BIOSCREEN has the following limitations:

1. **As an analytical model, BIOSCREEN assumes simple groundwater flow conditions.**

The model should not be applied where pumping systems create a complicated flow field. In addition, the model should not be applied where vertical flow gradients affect contaminant transport.

2. **As an screening tool, BIOSCREEN only approximates more complicated processes that occur in the field.**

The model should not be applied where extremely detailed, accurate results that closely match site conditions are required. More comprehensive numerical models should be applied in these cases.

FUNDAMENTALS OF NATURAL ATTENUATION

Biodegradation Modeling

Naturally occurring biological processes can significantly enhance the rate of organic mass removal from contaminated aquifers. Biodegradation research performed by Rice University, government agencies, and other research groups has identified several main themes that are crucial for future studies of natural attenuation:

1. *The relative importance of groundwater transport vs. microbial kinetics is a key consideration for developing workable biodegradation expressions in models. Results from the United Creosote site (Texas) and the Traverse City Fuel Spill site (Michigan) indicate that biodegradation is better represented as a macro-scale wastewater treatment-type process than as a micro-scale study of microbial reactions.*

2. *The distribution and availability of electron acceptors control the rate of in-situ biodegradation for most petroleum release site plumes. Other factors (e.g., population of microbes, pH, temperature, etc.) rarely limit the amount of biodegradation occurring at these sites.*

Borden *et al.* (1986) developed the BIOPLUME model, which simulates aerobic biodegradation as an "instantaneous" microbial reaction that is limited by the amount of electron acceptor,

oxygen, that is available. In other words, the microbial reaction is assumed to occur at a much faster rate than the time required for the aquifer to replenish the amount of oxygen in the plume. Although the time required for the biomass to aerobically degrade the dissolved hydrocarbons is on the order of days, the overall time to flush a plume with fresh groundwater is on the order of years or tens of years. Borden et al. (1986) incorporated a simplifying assumption that the microbial kinetics are instantaneous into the USGS two-dimensional solute transport model (Konikow and Bredehoeft, 1978) using a simple superposition algorithm. The resulting model, BIOPLUME, was able to simulate solute transport and fate under the effects of instantaneous, oxygen-limited in-situ biodegradation.

Rifai and Bedient (1990) extended this approach and developed the BIOPLUME II model, which simulates the transport of two plumes: an oxygen plume and a contaminant plume. The two plumes are allowed to react, and the ratio of oxygen to contaminant consumed by the reaction is determined from an appropriate stoichiometric model. The BIOPLUME II model is documented with a detailed user's manual (Rifai et al., 1987) and is currently being used by EPA regional offices, U.S. Air Force facilities, and by consulting firms. Borden et al. (1986) applied the BIOPLUME concepts to the Conroe Superfund site; Rifai et al. (1988) and Rifai et al. (1991) applied the BIOPLUME II model to a jet fuel spill at a Coast Guard facility in Michigan. Many other studies using the BIOPLUME II model have been presented in recent literature.

The BIOPLUME II model has increased the understanding of biodegradation and natural attenuation by simulating the effects of adsorption, dispersion, and aerobic biodegradation processes in one model. It incorporates a simplified mechanism (first-order decay) for handling other degradation processes, but does not address specific anaerobic decay reactions. Early conceptual models of natural attenuation were based on the assumption that the anaerobic degradation pathways were too slow to have any meaningful effect on the overall natural attenuation rate at most sites. Accordingly, most field programs focused only on the distribution of oxygen and contaminants, and did not measure the indicators of anaerobic activity such as depletion of anaerobic electron acceptors or accumulation of anaerobic metabolic by-products.

The Air Force Natural Attenuation Initiative

Over the past several years, the high cost and poor performance of many pump-and-treat remediation systems have led many researchers to consider RNA as an alternative technology for groundwater remediation. A detailed understanding of natural attenuation processes is needed to support the development of this remediation approach. Researchers associated with the U.S. EPA's R.S. Kerr Environmental Research Laboratory (now the Subsurface Protection and Remediation Division of the National Risk Management Laboratory) have suggested that anaerobic pathways could be a significant, or even the dominant, degradation mechanism at many petroleum fuel sites (Wilson, 1994). The natural attenuation initiative, developed by the AFCEE Technology Transfer Division, was designed to investigate how natural attenuation processes affect the migration of plumes at petroleum release sites. Under the guidance of Lt. Col. Ross Miller, a three-pronged technology development effort was launched in 1993 which will ultimately consist of the following elements:

1) *Field data collected at over 30 sites around the country (Wiedemeier, Miller, et al., 1995) analyzing aerobic and anaerobic processes.*

2) *A Technical Protocol, outlining the approach, data collection techniques, and data analysis methods required for conducting an Air Force RNA Study (Wiedmeier, Wilson, et al., 1995).*

3) *Two RNA modeling tools: the BIOPLUME III model being developed by Dr. Hanadi Rifai at Rice University (Rifai et al., 1995), and the BIOSCREEN model developed by*

Groundwater Services, Inc. (BIOPLUME III, a more sophisticated biodegradation model than BIOSCREEN, employs particle tracking of both hydrocarbon and alternate electron acceptors using a numerical solver. The model employs sequential degradation of the biodegradation reactions based on zero order, first order, instantaneous, or Monod kinetics).

Relative Importance of Different Electron Acceptors

The Intrinsic Remediation Technical Protocol and modeling tools focus on evaluating both aerobic (in the presence of oxygen) and anaerobic (without oxygen) degradation processes. In the presence of organic substrate and dissolved oxygen, microorganisms capable of aerobic metabolism will predominate over anaerobic forms. However, dissolved oxygen is rapidly consumed in the interior of contaminant plumes, converting these areas into anoxic (low-oxygen) zones. Under these conditions, anaerobic bacteria begin to utilize other electron acceptors to metabolize dissolved hydrocarbons. The principal factors influencing the utilization of the various electron acceptors by fuel-hydrocarbon-degrading bacteria include· 1) the relative biochemical energy provided by the reaction, 2) the availability of individual or specific electron acceptors at a particular site, and 3) the kinetics (rate) of the microbial reaction associated with the different electron acceptors.

Preferred Reactions by Energy Potential

Biologically mediated degradation reactions are reduction/oxidation (redox) reactions, involving the transfer of electrons from the organic contaminant compound to an electron acceptor. Oxygen is the electron acceptor for aerobic metabolism, whereas nitrate, ferric iron, sulfate, and carbon dioxide can serve as electron acceptors for alternative anaerobic pathways. This transfer of electrons releases energy which is utilized for microbial cell maintenance and growth. The biochemical energy associated with alternative degradation pathways can be represented by the redox potential of the alternative electron acceptors: the more positive the redox potential, the more energetically favorable the reaction. With everything else being equal, organisms with more efficient modes of metabolism grow faster and therefore dominate over less efficient forms.

Electron Acceptor	Type of Reaction	Metabolic By-Product	Redox Potential (pH = 7, in mvolts)*	Reaction Preference
Oxygen	Aerobic	CO_2	+ 820	*Most Preferred*
Nitrate	Anaerobic	N_2, CO_2	+ 740	⇓
Ferric Iron (solid)	Anaerobic	Ferrous Iron (dissolved)	- 50	⇓
Sulfate	Anaerobic	H_2S	- 220	⇓
Carbon Dioxide	Anaerobic	Methane	- 240	*Least Preferred*

* from Wiedemeier, Wilson, et al., 1995.

Based solely on thermodynamic considerations, the most energetically preferred reaction should proceed in the plume until all of the required electron acceptor is depleted. At that point, the next most-preferred reaction should begin and continue until that electron acceptor is consumed, leading to a pattern where preferred electron acceptors are consumed one at a time, in sequence. Based on this principle, one would expect to observe monitoring well data with "no detect" results for the more energetic electron acceptors, such as oxygen and nitrate, in locations

where evidence of less energetic reactions is observed (e.g. monitoring well data indicating the presence of ferrous iron).

In practice, however, it is unusual to collect samples from monitoring wells that are completely depleted in one or more electron acceptors. Two processes are probably responsible for this observation:

1. *Alternative biochemical mechanisms exhibiting very similar energy potentials (such as aerobic oxidation and nitrate reduction) may occur concurrently when the preferred electron acceptor is reduced in concentration, rather than fully depleted. Facultative aerobes (bacteria able to utilize electron acceptors in both aerobic and anaerobic environments), for example, can shift from aerobic metabolism to nitrate reduction when oxygen is still present but at low concentrations (i.e. 1 mg/L oxygen; Snoeyink and Jenkins, 1980). Similarly, ncting the nearly equivalent redox potentials for sulfate and carbon dioxide (-220 millivolts and -240 millivolts, respectively) one might expect that sulfate reduction and methanogenic reactions may also occur together.*

2. *Standard monitoring wells, with 5- to 10- foot screened intervals, will mix waters from different vertical zones. If different biodegradation reactions are occurring at different depths, then one would expect to find geochemical evidence of alternative degradation mechanisms occurring in the same well. If the dissolved hydrocarbon plume is thinner than the screened interval of a monitoring well, then the geochemical evidence of electron acceptor depletion or metabolite accumulation will be diluted by mixing with clean water from zones where no degradation is occurring.*

Therefore, most natural attenuation programs yield data that indicate a general pattern of electron acceptor depletion, but not complete depletion, and an overlapping of electron acceptor/metabolite isopleths into zones not predicted by thermodynamic principles. For example, a zone of methane accumulation may be larger than the apparent anoxic zone. Nevertheless, these general patterns of geochemical changes within the plume area provide strong evidence that multiple mechanisms of biodegradation are occurring at many sites. The BIOSCREEN software attempts to account for the majority of these biodegradation mechanisms.

Distribution of Electron Acceptors at Sites

The utilization of electron acceptors is generally based on the energy of the reaction and the availability of the electron acceptor at the site. While the energy of each reaction is based on thermodynamics, the distribution of electron acceptors is dependent on site-specific hydrogeochemical processes and can vary significantly among sites. For example, a study of several sites yielded the following summary of available electron acceptors and metabolic by-products:

Measured Background Electron Acceptor/By-Product Concentration (mg/L)					
Base Facility	Background Oxygen	Background Nitrate	Maximum Ferrous Iron	Background Sulfate	Maximum Methane
POL Site, Hill AFB, Utah*	6.0	36.2	55.6	96.6	2.0
Hangar 10 Site, Elmendorf AFB, Alaska*	0.8	64.7	8.9	25.1	9.0
Site ST-41, Elmendorf AFB, Alaska*	12.7	60.3	40.5	57.0	1.5
Site ST-29, Patrick AFB, Florida*	3.8	0	2.0	0	13.6
Bldg. 735, Grissom AFB, Indiana	9.1	1.0	2.2	59.8	1.0
SW MU 66 Site, Keesler AFB, MS	1.7	0.7	36.2	22.4	7.4
POL B Site, Tyndall AFB, Florida	1.4	0.1	1.3	5.9	4.6

*Data collected by Parsons Engineering Science. Inc.; all other data collected by Groundwater Services. Inc.

At the Patrick AFB site, nitrate and sulfate are not important electron acceptors while the oxygen and the methanogenic reactions dominate (Wiedemeier, Swanson, et al., 1995). At Hill AFB and Grissom AFB, the sulfate reactions are extremely important because of the large amount of available sulfate for reduction. Note that different sites in close proximity can have quite different electron acceptor concentrations, as shown by the two sites at Elmendorf AFB. For data on more sites, see Table 1.

Kinetics of Aerobic and Anaerobic Reactions

As described above, aerobic biodegradation can be simulated as an "instantaneous" reaction that is limited by the amount of electron acceptor (oxygen) that is available. The microbial reaction is assumed to occur at a much faster rate than the time required for the aquifer to replenish the amount of oxygen in the plume (Wilson et al., 1985). Although the time required for the biomass to aerobically degrade the dissolved hydrocarbons is on the order of days, the overall time to flush a plume with fresh groundwater is on the order of years or tens of years.

For example, microcosm data presented by Davis et al. (1994) show that microbes in an environment with an excess of electron acceptors can degrade high concentrations of dissolved benzene very rapidly. In the presence of surplus oxygen, aerobic bacteria can degrade ~1 mg/L dissolved benzene in about 8 days, which can be considered relatively fast (referred to as "instantaneous") compared to the years required for flowing groundwater to replenish the plume area with oxygen.

TABLE 1
BIODEGRADATION CAPACITY (EXPRESSED ASSIMILATIVE CAPACITY) AT AFCEE NATURAL ATTENUATION SITES
BIOSCREEN Natural Attenuation Decision Support System

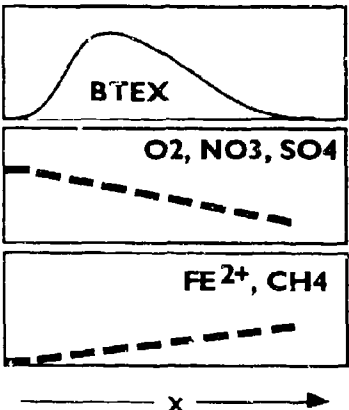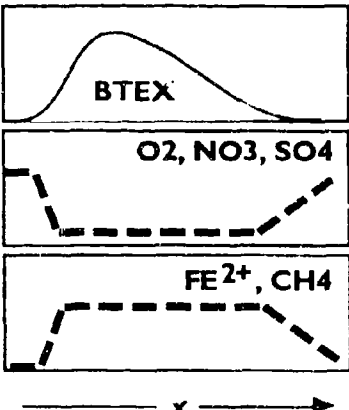| Site Number	Base	State	Site Name	Maximum Total BTEX Concentration (mg/L)	Observed Change in Concentration (mg/L)					Biodegradation Capacity/Expressed Assimilative Capacity (mg/L)					Total Biodegradation Capacity (mg/L)	Source of Data
					O2	Nitrate	Iron	Sulfate	Methane	Aerobic Respiration	Denitrification	Iron Reduction	Sulfate Reduction	Methanogenesis		
1	Hill AFB	Utah		21.5	6.0	36.2	55.6	96.6	2.0	1.9	7.4	2.6	21.0	2.6	35.4	PES
2	Battle Creek ANGB	Michigan		3.6	5.7	5.6	12.0	12.9	8.4	1.8	1.1	0.6	2.8	10.5	17.1	PES
3	Madison ANGB	Wisconsin		28.0	7.2	45.3	15.3	24.2	11.7	2.3	9.2	0.7	5.3	15.0	32.5	PES
4	Elmendorf AFB	Alaska	Hangar 10	22.2	0.8	64.7	9.9	25.1	9.0	0.3	13.2	0.4	5.5	11.6	30.9	PES
5	Elmendorf AFB	Alaska	ST-41	30.6	12.7	60.3	40.5	57.0	1.5	4.0	12.3	1.4	12.4	1.9	32.5	PES
6	King Salmon AFB	Alaska	FT-001	10.1	9.0	12.5	2.5	6.8	0.2	2.9	2.6	0.1	1.5	0.2	7.2	PES
7	King Salmon AFB	Alaska	Nabesk	5.3	11.7	0	44.0	0	5.6	3.7	0	2.0	0	7.2	12.9	PES
8	Plattsburgh AFB	New York		6.0	10.0	3.7	10.7	18.9	0.3	3.2	0.7	0.5	4.1	0.4	8.9	PES
9	Eglin AFB	Florida		3.7	1.2	0	8.9	4.9	11.8	0.4	0	0.4	1.1	15.2	17.0	PES
10	Patrick AFB	Florida		7.3	3.8	0	2.0	0	13.6	1.2	0	0.1	0	17.4	18.7	PES
11	MacDill AFB	Florida	Site 56	29.6	2.4	5.6	5.0	101.2	13.6	0.8	1.1	0.2	22.0	17.4	41.5	PES
12	MacDill AFB	Florida	Site 57	0.7	2.1	0.5	20.9	62.4	15.4	0.7	0.1	1.0	13.6	19.7	35.0	PES
13	MacDill AFB	Florida	Site OT-24	2.8	1.3	0	13.1	3.7	9.8	0.4	0	0.6	0.8	12.6	14.4	PES
14	Offutt AFB	Nebraska	FPT-A3	3.2	0.6	0	19.0	32.0	22.4	0.2	0	0.9	7.0	28.8	36.8	PES
15	Offutt AFB	Nebraska		103.0	8.4	69.7	?	82.9	0	2.7	14.2	0	18.0	0	34.9	PES
16	Westover AFRES	Massachusetts	FT-03	1.7	10.0	8.6	599.5	33.5	0.2	3.2	1.8	27.5	7.3	0.2	40.0	PES
17	Westover AFRES	Massachusetts	FF-08	32.6	9.9	17.2	279.0	11.7	4.3	3.1	3.5	12.8	2.6	5.5	27.5	PES
18	Myrtle Beach	South Carolina		18.3	0.4	0	34.9	20.7	17.2	0.1	0	1.6	4.5	22.0	28.2	PES
19	Langley AFB	Virginia		0.1	6.4	23.5	10.9	61.3	8.0	2.0	4.8	0.5	17.7	10.2	35.3	PES
20	Griffis AFB	New York		12.6	4.4	52.5	24.7	82.2	7.1	1.4	10.7	1.1	17.9	9.1	40.2	PES
21	Rickenbacker ANGB	Ohio		1.0	1.5	35.9	17.9	93.2	7.7	0.5	7.3	0.8	20.3	9.8	38.7	PES
22	Wurtsmith AFB	Michigan	SS-42	3.1	8.5	25.4	19.9	10.6	1.4	2.7	5.2	0.9	2.3	1.8	12.9	PES
23	Travis AFB	California			3.8	15.8	8.5	109.2	0.2	1.2	3.2	0.4	23.7	0.3	28.5	PES
24	Pope AFB	North Carolina		8.2	7.5	6.9	56.2	9.7	48.4	2.4	1.4	2.6	2.1	62.0	70.5	PES
25	Seymour Johnson AFB	North Carolina		13.8	8.3	4.3	31.6	38.6	2.7	2.6	0.9	1.5	8.4	3.5	16.8	PES
26	Grissom AFB	Indiana	Bldg 735	0.3	9.1	1.0	2.2	59.8	1.0	2.9	0.2	0.1	13.0	1.2	17.4	GSI
27	Tyndall AFB	Florida	POL B	1.0	1.4	0.1	1.7	5.9	4.6	0.5	0	0.1	1.3	5.9	7.7	GSI
28	Keesler AFB	Mississippi	SWMU 66	14.1	1.7	0.7		22.4	7.4	0.5	0.1	1.7	4.9	9.5	16.7	GSI
			Average	14.2	5.6	17.7	49.3	39.5	8.4	1.8	3.6	2.3	8.6	10.8	27.0	
			Median	7.3	5.8	6.3	16.6	74.6	7.2	1.9	1.3	0.8	5.4	9.3	28.5	
			Maximum	103.0	12.7	69.7	599.5	109.2	48.4	4.0	14.2	27.5	23.7	62.0	70.5	
			Minimum	0.1	0.4	0	0	0	0	0.1	0	0	0	0	7.2	

Note
1 Utilization factors of the electron acceptors/by-products are as follows (mg of electron acceptor or by-product/mg of BTEX)   Dissolved Oxygen 3.14, Nitrate 4.9, Iron 21.8, Sulfate 4.7, Methane 0.78
2 - = Data not available
3 PES = Parsons Engineering Science (Wiedemeier, Miller, et al 1995)   GSI = Groundwater Services, Inc

Recent results from the AFCEE Natural Attenuation Initiative indicate that the anaerobic reactions, which were originally thought to be too slow to be of significance in groundwater, can also be simulated as instantaneous reactions (Newell et al., 1995). For example, Davis et al. (1994) also ran microcosm studies with sulfate reducers and methanogens that indicated that benzene could be degraded in a period of a few weeks (after acclimation). When compared to the time required to replenish electron acceptors in a plume, it appears appropriate to simulate anaerobic biodegradation of dissolved hydrocarbons with an instantaneous reaction, just as for aerobic biodegradation processes.

This conclusion is supported by observing the pattern of anaerobic electron acceptors and metabolic by-products along the plume at RNA research sites:

If microbial kinetics were limiting the rate of biodegradation:	If microbial kinetics were relatively fast (instantaneous):
• Anaerobic electron acceptors (nitrate and sulfate) would be constantly **decreasing** in concentration as one moved downgradient from the source zone, and	• Anaerobic electron acceptors (nitrate and sulfate) would be mostly or totally consumed in the source zone, and
• Anaerobic by-products (ferrous iron and methane) would be constantly **increasing** in concentration as one moved downgradient from the source zone.	• Anaerobic by-products (ferrous iron and methane) would be found in the highest concentrations in the source zone.

The second pattern is observed at RNA demonstration sites (see Figure 1), supporting the hypothesis that anaerobic reactions can be considered to be relatively instantaneous at most or almost all petroleum release sites. From a theoretical basis, the only sites where the instantaneous reaction assumption may not apply are sites with very low hydraulic residence times (very high groundwater velocities and short source zone lengths).
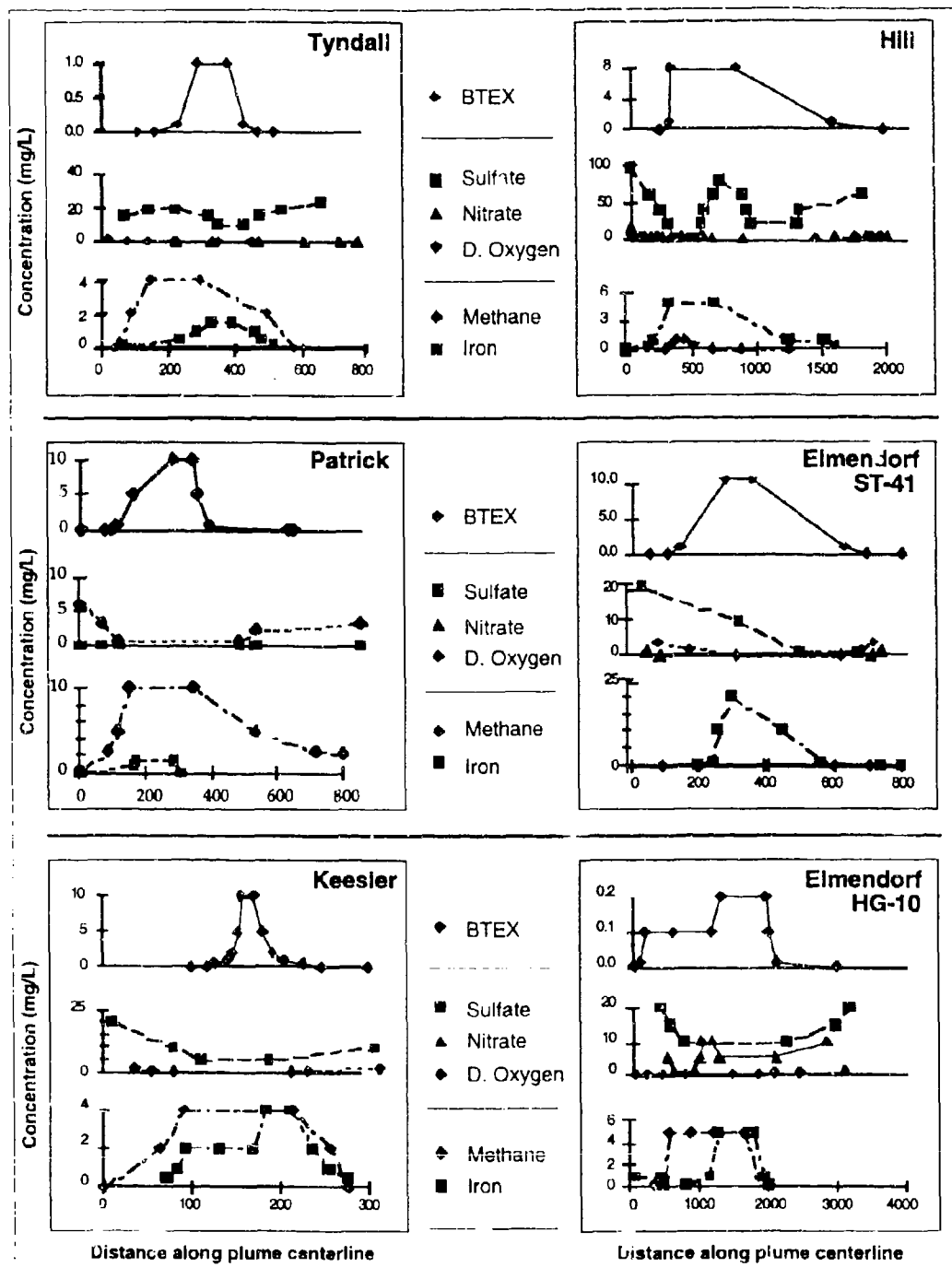
Figure 1. Distribution of BTEX, Electron Acceptors, and Metabolic By-Products vs. Distance Along Centerline of Plume.

Sampling Date and Source of Data: Tyndall 3/95 , Keesler 4/95 (Groundwater Services, Inc.), Patrick 3/94 (note: 1 NO3 outlier removed, sulfate not plotted), Hill 7/93, Elmendorf Site ST41 6/94, Elmendorf Site HG 10 6/94, (Parsons Engineering Science).

Kinetic-limited sites, however, appear to be relatively rare as the instantaneous reaction pattern is observed even at sites such as Site 870 at Hill AFB, with residence times of a month or less. As shown in Figure 1, this site has an active sulfate reducing and methane production zone within 100 ft of the upgradient edge of plume. With a 1600 ft/yr seepage velocity is considered, this highly anaerobic zone has an effective residence time of 23 days. Despite this very short residence time, significant sulfate depletion and methane production were observed in this zone (see Figure 1). If the anaerobic reactions were significantly constrained by microbial kinetics, the amount of sulfate depletion and methane production would be much less pronounced. Therefore this site supports the conclusion that the instantaneous reaction assumption is applicable to almost all petroleum release sites.

Biodegradation Capacity

To apply an electron-acceptor-limited kinetic model, such as the instantaneous reaction, the amount of biodegradation able to be supported by the groundwater that moves through the source zone must be calculated. The conceptual model used in BIOSCREEN is:

1. Groundwater upgradient of the source contains electron acceptors.

2. As the upgradient groundwater moves through the source zone, non-aqueous phase liquids (NAPLs) and contaminated soil release dissolvable hydrocarbons (in the case of petroleum sites, the BTEX compounds benzene, toluene, ethylbenzene, xylene are released).

3. Biological reactions occur until the available electron acceptors in groundwater are consumed. (Two exceptions to this conceptual model are the iron reactions, where the electron acceptor, ferric iron, dissolves from the aquifer matrix; and the methane reactions, where the electron acceptor, CO_2 is also produced as an end-product of the reactions. For these reactions, the metabolic by-products, ferrous iron and methane, can be used as proxies for the potential amount of biodegradation that could occur from the iron-reducing and methanogenesis reactions.)

4. The total amount of available electron acceptors for biological reactions can be estimated by a) calculating the difference between upgradient concentrations and source zone concentrations for oxygen, nitrate, and sulfate; and b) measuring the production of metabolic by-products (ferrous iron and methane) in the source zone.

5. Using stoichiometry, a utilization factor can be developed showing the ratio of the oxygen, nitrate, and sulfate consumed to the mass of dissolved hydrocarbon degraded in the biodegradation reactions. Similarly, utilization factors can be developed to show the ratio of the mass of metabolic by-products that are generated to the mass of dissolved hydrocarbon degraded in the biodegradation reactions. Wiedemeier, Wilson, et al., (1995) provides the following utilization factors based on the degradation of combined BTEX constituents:

Electron Acceptor/By-Product	BTEX Utilization Factor gm/gm
Oxygen	3.14
Nitrate	4.9
Ferrous Iron	21.8
Sulfate	4.7
Methane	0.78

6. For a given background concentration of an individual electron acceptor, the potential contaminant mass removal or "biodegradation capacity" depends on the "utilization factor" for that electron acceptor. Dividing the background concentration of an electron acceptor by its utilization factor provides an estimate (in BTEX concentration units) of the assimilative capacity of the aquifer by that mode of biodegradation.

Note that BIOSCREEN is based on the BTEX utilization provided above. If other constituents are modeled, the utilization factors in the software (scroll down from the input screen to find the utilization factors) should be changed or the available oxygen, nitrate, iron, sulfate, and methane data should be adjusted accordingly to reflect alternate utilization factors.

When the available electron acceptor/by-product concentrations (No. 4) are divided by the appropriate utilization factor (No. 5), an estimate of the "biodegradation capacity" of the groundwater flowing through the source zone and plume can be developed. The biodegradation capacity is then used directly in the BIOSCREEN model to simulate the effects of an instantaneous reaction. The suggested calculation approach to develop BIOSCREEN input data is:

Biodegradation Capacity (mg/L) =

{ (Average Upgradient Oxygen Conc.) - (Minimum Source Zone Oxygen Conc) } / 3.14

+   { (Average Upgradient Nitrate Conc.) - (Minimum Source Zone Nitrate Conc) } /4.9

+   { (Average Upgradient Sulfate Conc.) - (Minimum Source Zone Sulfate Conc) } / 4.7

+   { Average Observed Ferrous Ion Conc. in Source Area} / 21.8

+   { Average Observed Methane Conc. in Source Area } / 0.78

Biodegradation capacity is similar to "Expressed Assimilative Capacity" (EAC) described in the AFCEE Technical Protocol except that EAC calculations do not use the maximum source concentrations for iron and methane. Calculated biodegradation capacities or EACs at different U.S. Air Force RNA research sites have ranged from 7 to 70 mg/l. (see Table 1). The median biodegradation capacity/EAC for 28 AFCEE sites is 28.5 mg/l.

Note that one criticism of this lumped biodegradation capacity approach is that it assumes that all of the various aerobic and anaerobic reactions occur over the entire area of the contaminant plume, and that the theoretical "zonation" of reactions is not simulated in BIOSCREEN (e.g. typically dissolved oxygen utilization occurs at the downgradient portion and edges of the plume, nitrate utilization a little closer to the source, iron reduction in the middle of the plume, sulfate reduction near the source, and methane production in the heart of the source zone). A careful inspection of actual field data (see Figure 1) shows little or no evidence of this theoretical zonation of reactions; in fact all of the reactions appear to occur simultaneously in the source zone. The most common pattern observed at petroleum release sites is that ferrous iron seems to be restricted to the higher-concentration or source zone areas, with the other reactions (oxygen, nitrate, and sulfate depletion), occurring throughout the plume.

BIOSCREEN assumes that all of the biodegradation reactions (aerobic and anaerobic) occur almost instantaneously relative to the hydraulic residence time in the source area and plume. Because iron reduction and methane production appear to occur only in the source zone (probably due to the removal of these metabolic by-products) it is recommended to use the *average* iron and methane concentrations observed in the source

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zone for the calculation of biodegradation capacity instead of maximum concentrations. In addition, the iron and methane concentrations are used during a secondary calibration step (see below). Beta testing of BIOSCREEN indicated that the use of the maximum concentration of iron and methane tended to overpredict biodegradation at many sites by assuming these reactions occurred over the entire plume area. Use of an average value (or some reduced value) helps match actual field data.

7. Note that at some sites the instantaneous reaction model will appear to overpredict the amount of biodegradation that occurs, and underpredict at others. As with the case of the first-order decay model, some calibration to actual site conditions is required. With the first-order decay, the decay coefficient is adjusted arbitrarily until the predicted values match observed field conditions. With the instantaneous reaction model, there is no first-order decay coefficient to adjust, so the following procedure is recommended:

    A) The primary calibration step (if needed) is to manipulate the model's dispersivity values. As described in the BIOSCREEN Data Entry Section below, values for dispersivity are related to aquifer scale (defined as the plume length or distance to the measurement point) and simple relationships are usually applied to estimate dispersivities. Gelhar *et al.* (1992) cautions that dispersivity values vary between 2-3 orders of magnitude for a given scale due to natural variation in hydraulic conductivity at a particular site. Therefore dispersivity values can be manipulated within a large range and still be within the range of values observed at field test sites. In BIOSCREEN, adjusting the transverse dispersivity alone will usually be enough to calibrate the model.

    B) As a secondary calibration step, the biodegradation capacity calculation may be reevaluated. There is some judgment involved in averaging the electron acceptor concentrations observed in upgradient wells; determining the minimum oxygen, nitrate and sulfate in the source zone; and estimating the average ferrous iron and methane concentrations in the source zone. Although probably not needed in most applications, these values may be adjusted as a final level of calibration.

BIOSCREEN CONCEPTS

The BIOSCREEN Natural Attenuation software is based on the Domenico (1987) three-dimensional analytical solute transport model. The original model assumes a fully-penetrating vertical plane source oriented perpendicular to groundwater flow, to simulate the release of organics to moving groundwater. In addition, the Domenico solution accounts for the effects of advective transport, three-dimensional dispersion, adsorption, and first-order decay. In BIOSCREEN, the Domenico solution has been adapted to provide three different model types representing i) transport with no decay, ii) transport with first-order decay, and iii) transport with "instantaneous" biodegradation reaction (see Model Types). Guidelines for selecting key input parameters for the model are outlined in BIOSCREEN Input Parameters. For help on Output, see BIOSCREEN Output.

BIOSCREEN Model Types

The software allows the user to see results from three different types of groundwater transport models, all based on the Domenico solution:

1. **Solute transport with no decay.** This model is appropriate for predicting the movement of conservative (non-degrading) solutes such as chloride. The only attenuation mechanisms are dispersion in the longitudinal, transverse, and vertical directions, and adsorption of contaminants to the soil matrix.

2. **Solute transport with first-order decay.** With this model, the solute degradation rate is proportional to the solute concentration. The higher the concentration, the higher the degradation rate. This is a conventional method for simulating biodegradation in dissolved hydrocarbon plumes. Modeler using the first-order decay model typically use the first-order decay coefficient as a calibration parameter, and adjust the decay coefficient until the model results match field data. With this approach, uncertainties in a number of parameters (e.g., dispersion, sorption, biodegradation) are lumped together in a single calibration parameter.

   Literature values for the half-life of benzene, a readily biodegradable dissolved hydrocarbon, range from 10 to 730 days while the half-life for TCE, a more recalcitrant constituent, is 10.7 months to 4.5 years (Howard *et al.*, 1991). Other applications of the first-order decay approach include radioactive solutes and abiotic hydrolysis of selected organics, such as dissolved chlorinated solvents. One of the best sources of first-order decay coefficients in groundwater systems is *The Handbook of Environmental Degradation Rates* (Howard *et al.*, 1991).

   The first-order decay model does not account for site-specific information such as the availability of electron acceptors. In addition, it does not assume any biodegradation of dissolved constituents in the source zone. In other words, this model assumes biodegradation starts immediately downgradient of the source, and that it does not depress the concentrations of dissolved organics in the source zone itself.

3. **Solute transport with "instantaneous" biodegradation reaction.** Modeling work conducted by GSI indicate first-order expressions may not be as accurate for describing natural attenuation processes as the instantaneous reaction assumption (Connor *et al.*, 1994). Biodegradation of organic contaminants in groundwater is more difficult to quantify using a first-order decay equation because electron acceptor limitations are not considered. A more accurate prediction of biodegradation effects may be realized by incorporating the instantaneous reaction equation into a transport model. This approach forms the basis for the BIOSCREEN instantaneous reaction model.

   To incorporate the instantaneous reaction in BIOSCREEN, a superposition method was used. By this method, contaminant mass concentrations at any location and time within the flow field are corrected by subtracting 1 mg/L organic mass for each mg/L of biodegradation capacity provided by all of the available electron acceptors, in accordance with the instantaneous reaction assumption. Borden *et al.* (1986) concluded that this simple superposition technique was an exact replacement for more sophisticated oxygen-limited expressions, as long as the oxygen and hydrocarbon had the same transport rates (e.g., retardation factor, R = 1). Connor *et al.* (1994) revived this approach for use in spreadsheets and compared the results to those from more sophisticated but difficult to use numerical models. They found this approach to work well, even for retardation factors greater than 1, so this superposition approach was incorporated into the BIOSCREEN model (see Appendix A.2).

Which Kinetic Model Should One Use in BIOSCREEN?

BIOSCREEN gives the user three different models to choose from to help see the effect of biodegradation. At almost all petroleum release sites, biodegradation is present and can be verified by demonstrating the consumption of aerobic and anaerobic electron acceptors. Therefore, results from the No Biodegradation model are intended only to be used for comparison purposes and to demonstrate the effects of biodegradation on plume migration.

Some key factors for comparison of the First-order Decay model and the Instantaneous Reaction model are presented below:

FACTOR	First-Order Decay Model	Instantaneous Reaction Model
Able to Utilize Data from AFCEE Intrinsic Remediation Protocol?	• *No - Does not account for electron acceptors/by-products*	• *Yes - Accounts for availability of electron acceptors and by-products*
Simple to Use?	• *Yes*	• *Yes*
Simplification of Numerical Model?	• *Yes - many numerical models include first-order decay*	• *Yes - Simplification of BIOPLUME III model*
Familiar to Modelers?	• *More commonly used*	• *Used less frequently*
Key Calibration Parameter	• *First-Order Decay Coefficients*	• *Source Term/Dispersivity*
Over - or Underestimates Source Decay Rate?	• *May underpredict rate of source depletion (see Newell et al., 1995)*	• *May be more accurate for estimating rate of source depletion (see Newell et al., 1995)*

A key goal of the AFCEE Natural Attenuation Initiative is to quantify the magnitude of RNA based on field measurements of electron acceptor consumption and metabolic by-product production. Therefore, the Instantaneous Reaction model is recommended either alone or in addition to the first-order decay model (if appropriate calibration is performed) for most sites where the Intrinsic Remediation Technical Protocol (Wiedemeier, Wilson, *et al.*, 1995) has been applied. For a more rigorous analysis of natural attenuation, the BIOPLUME III model (to be released in late 1996) may be more appropriate.

BIOSCREEN DATA ENTRY

Three important considerations regarding data input are:

1   To see the example data set in the input screen of the software, click on the "Paste Example Data Set" button on the lower right portion of the input screen.

2)   Because BIOSCREEN is based on the Excel spreadsheet, you have to click outside of the cell where you just entered data or hit "return" before any of the buttons will work.

3)   Several cells have data that can be entered directly or can be calculated by the model using data entered in the grey cells (e.g., seepage velocity can be entered directly or calculated using hydraulic conductivity, gradient, and effective porosity). If the calculation option does not appear to work, check to make sure that there is still a formula in the cell. If not, you can restore the formula by clicking on the "Restore Formulas" button on the bottom right hand side of the input screen. If there still appears to be a problem, click somewhere outside of the last cell where you entered data and then click on the "Recalculate" button on the input screen.

I. HYDROGEOLOGIC DATA

Parameter	Seepage Velocity (Vs)
Units	ft/yr
Description	Actual interstitial groundwater velocity, equaling Darcy velocity divided by effective porosity. Note that the Domenico model and BIOSCREEN are not formulated to simulate the effects of chemical diffusion. Therefore, contaminant transport through very slow hydrogeologic regimes (e.g., clays and slurry walls) should probably not be modeled using BIOSCREEN unless the effects of chemical diffusion are proven to be insignificant. Domenico and Schwartz (1990) indicate that chemical diffusion is insignificant for Peclet numbers (seepage velocity times median pore size divided by the bulk diffusion coefficient) > 100.
Typical Values	0.5 to 200 ft/yr
Source of Data	Calculated by multiplying hydraulic conductivity by hydraulic gradient and dividing by effective porosity. It is strongly recommended that actual site data be used for hydraulic conductivity and hydraulic gradient data parameters; effective porosity can be estimated.
How to Enter Data	1) Enter directly or 2) Fill in values for hydraulic conductivity, hydraulic gradient, and effective porosity as described below and have BIOSCREEN calculate seepage velocity. Note: if the calculation option does not appear to work, check to make sure that the cell still contains a formula. If not, you can reincarnate the formula by clicking on the "Restore Formulas" button on the bottom right hand side of the input screen. If there is still a problem, make sure to click somewhere outside of the last cell where you entered data and then click on the "Recalculate" button on the input screen.

Parameter	Hydraulic Conductivity (K)	
Units	cm/sec	
Description	Horizontal hydraulic conductivity of the saturated porous medium.	
Typical Values	Clays:	$<1 \times 10^{-6}$ cm/s
	Silts:	$1 \times 10^{-6} - 1 \times 10^{-3}$ cm/s
	Silty sands:	$1 \times 10^{-5} - 1 \times 10^{-1}$ cm/s
	Clean sands:	$1 \times 10^{-3} - 1$ cm/s
	Gravels:	>1 cm/s
Source of Data	Pump tests or slug tests at the site. It is strongly recommended that actual site data be used for most RNA studies.	
How to Enter Data	Enter directly. If seepage velocity is entered directly, this parameter is not needed in BIOSCREEN.	

Parameter	Hydraulic Gradient (i)
Units	ft/ft
Description	The slope of the potentiometric surface. In unconfined aquifers, this is equivalent to the slope of the water table.
Typical Values	0.0001 - 0.05 ft/ft
Source of Data	Calculated by constructing potentiometric surface maps using static water level data from monitoring wells and estimating the slope of the potentiometric surface.
How to Enter Data	Enter directly. If seepage velocity is entered directly, this parameter is not needed in BIOSCREEN.

Parameter	Effective Porosity (n)
Units	unitless
Description	Dimensionless ratio of the volume of interconnected voids to the bulk volume of the aquifer matrix. Note that "total porosity" is the ratio of all voids (included non-connected voids) to the bulk volume of the aquifer matrix. Difference between total and effective porosity reflect lithologic controls on pore structure. In unconsolidated sediments coarser than silt size, effective porosity can be less than total porosity by 2-5% (e.g. 0.28 vs, 0.30) (Smith and Wheatcraft, 1993).
Typical Values	Values for Effective Porosity: Clay 0.01 - 0.20 Sandstone 0.005 - 0.10 Silt 0.01 - 0.30 Unfract. Limestone 0.001 - 0.05 Fine Sand 0.10 - 0.30 Fract. Granite 0.00005 - 0.01 Medium Sand 0.15 - 0.30 Coarse Sand 0.20 - 0.35 Gravel 0.10 - 0.35 (From Wiedemeier, Wilson, (From Domenico and Schwartz, 1990) et al., 1995, originally from Domenico and Schwartz, 1990 and Walton, 1988)
Source of Data	Typically estimated. One commonly used value for silts and sands is an effective porosity of 0.25. The ASTM RBCA Standard (ASTM, 1995) includes a default value of 0.38 (to be used primarily for unconsolidated deposits).
How to Enter Data	Enter directly. Note that if seepage velocity is entered directly, this parameter is still needed to calculate the retardation factor and plume mass.

2. DISPERSIVITY

Parameter	Longitudinal Dispersivity (alpha x) Transverse Dispersivity (alpha y) Vertical Dispersivity (alpha z)
Units	ft
Description	Dispersion refers to the process whereby a plume will spread out in a longitudinal direction (along the direction of groundwater flow), transversely (perpendicular to groundwater flow), and vertically downwards due to mechanical mixing in the aquifer and chemical diffusion. Selection of dispersivity values is a difficult process, given the impracticability of measuring dispersion in the field. However, simple estimation techniques based on the length of the plume or distance to the measurement point ("scale") are available from a compilation of field test data. Note that researchers indicate that dispersivity values can range over 2-3 orders of magnitude for a given value of plume length or distance to measurement point (Gelhar et al., 1992). In BIOSCREEN, dispersivity is used as the primary calibration parameter (see pg 10). For more information on dispersivity, see Appendix A.3, pg 40).
Typical Values	Typical dispersivity relationships as a function of Lp (plume length or distance to measurement point in ft) are provided below. BIOSCREEN is programmed with some commonly used relationships representative of typical and low-end dispersivities.

• Longitudinal Dispersivity

$\text{Alpha } x = 3.28 \cdot 0.83 \left[\log_{10}\left(\frac{L_p}{3.28}\right)\right]^{2.414}$ (Xu and Eckstein, 1995)

$(L_p \text{ in ft})$

• Transverse Dispersivity

Alpha y = 0.10 alpha x   (Based on high reliability points from Gelhar et al., 1992)

• Vertical Dispersivity

Alpha z = very low (i.e. 1×10^{-99} ft)   (Based on conservative estimate)

Other commonly used relationships include:

Alpha x	0.1 Lp	(Pickens and Grisak, 1981)
Alpha y	0.33 alpha x	(ASTM, 1995) (EPA, 1986)
Alpha z	0.05 alpha x	(ASTM, 1995)
Alpha z	0.025 alpha x to 0.1 alpha x	(EPA, 1986)
Source of Data	Typically estimated using the relationships provided above (see Appendix A.3, pg 40)
How to Enter Data	1) Enter directly or 2) Fill in value of the estimated plume length and have BIOSCREEN calculate the dispersivities.

Parameter	Estimated Plume Length (Lp)
Units	f t
Description	Estimated length (in feet) of the existing or hypothetical groundwater plume being modeled. This is a key parameter as it is generally used to estimate the dispersivity terms (dispersivity is difficult to measure and field data are rarely collected).
Typical Values	For BTEX plumes, 50 - 500 ft. For chlorinated solvents, 50 to 1000 ft.
Source of Data	To simulate an actual plume length or calibrate to actual plume data, enter the actual length of the plume. If trying to predict the maximum extent of plume migration, use one of the two methods below. 1) Use seepage velocity, retardation factor, and simulation time to estimate plume length. While this may underestimate the plume length for a non-degrading solute, it may overestimate the plume length for either the first-order decay model or instantaneous reaction model if biodegradation is significant. 2) Estimate a plume length, run the model, determine how long the plume is predicted to become (this will vary depending on the type of kinetic expression that is used), reenter this value, and then rerun the model. Note that considerable time and effort can be expended trying to adjust the estimated plume length term to match exactly the predicted modeling length. In practice, most modelers make the assumption that dispersivity values are not very precise, and therefore select ball-park values based on estimated plume lengths that are probably ± 25% of the actual plume length used in the simulations. Note that BIOSCREEN is very sensitive to the dispersion estimates, particularly for the instantaneous reaction model.
How to Enter Data	Enter directly. If dispersivity data are entered directly, this parameter is not needed in BIOSCREEN.

3. ADSORPTION DATA

Parameter	Retardation Factor (R)
Units	unitless
Description	The rate at which dissolved contaminants moving through an aquifer can be reduced by sorption of contaminants to the solid aquifer matrix. The degree of retardation depends on both aquifer and constituent properties. The retardation factor is the ratio of the groundwater seepage velocity to the rate that organic chemicals migrate in the groundwater. A retardation value of 2 indicates that if the groundwater seepage velocity is 100 ft/yr, then the organic chemicals migrate at approximately 50 ft/yr.
	BIOSCREEN simulations using the instantaneous reaction assumption at sites with retardation factors greater than 6 should be performed with caution and verified using a more sophisticated model such as BIOPLUME III (see Appendix A.2).
Typical Values	1 to 2 (for BTEX in typical shallow aquifer)
Source of Data	Usually estimated from soil and chemical data using variables described below (pb = bulk density, n = porosity, Koc = organic carbon-water partition coefficient, Kd = distribution coefficient, and foc = fraction organic carbon on uncontaminated soil) with the following expression:
	$$R = 1 + \frac{K_d \cdot \rho_b}{n} \qquad \text{where} \quad K_d = K_{oc} \cdot f_{oc}$$
	In some cases, the retardation factor can be estimated by comparing the length of a plume affected by adsorption (such as the benzene plume) with the length of plume that is not affected by adsorption (such as chloride). Most plumes do not have both types of contaminants, so it is more common to use the estimation technique (see data entry boxes below).
How to Enter Data	1) Enter directly or 2) Fill in the estimated values for bulk density, partition coefficient, and fraction organic carbon as described below and have BIOSCREEN calculate retardation.

Parameter	Soil Bulk Density (ρ_b)
Units	kg/L or g/cm^3
Description	Bulk density, in kg/L, of the aquifer matrix (related to porosity and pure solids density).
Typical Values	Although this value can be measured in the lab, in most cases estimated values are used. A value of 1.7 kg/L is used frequently.
Source of Data	Either from an analysis of soil samples at a geotechnical lab or more commonly, application of estimated values such as 1.7 kg/L.
How to Enter Data	Enter directly. If the retardation factor is entered directly, this parameter is not needed in BIOSCREEN.

Parameter	Organic Carbon Partition Coefficient (Koc)		
Units	(mg/kg) / (mg/L) or (L/kg) or (mL/g)		
Description	Chemical-specific partition coefficient between soil organic carbon and the aqueous phase. Larger values indicate greater affinity of contaminants for the organic carbon fraction of soil. This value is chemical specific and can be found in chemical reference books. Note that many users of BIOSCREEN will simulate BTEX as a single constituent. In this case, either an average value for the BTEX compounds can be used, or it can be assumed that all of the BTEX compounds have the same mobility as benzene (the constituent with the highest potential risk to human health).		
Typical Values	Benzene 38 L/kg Ethylbenzene 95 L/kg Toluene 135 L/kg Xylene 240 L/kg (ASTM, 1995) (Note that there is a wide range of reported values; for example, Mercer and Cohen (1990) report a Koc for benzene of 83 L/kg.		
Source of Data	Chemical reference literature or relationships between Koc and solubility or Koc and the octanol-water partition coefficient (Kow).		
How to Enter Data	Enter directly. If the retardation factor is entered directly, this parameter is not needed in BIOSCREEN.		

Parameter	Fraction Organic Carbon (foc)		
Units	unitless		
Description	Fraction of the aquifer soil matrix comprised of natural organic carbon in uncontaminated areas. More natural organic carbon means higher adsorption of organic constituents on the aquifer matrix.		
Typical Values	0.0002 - 0.02		
Source of Data	The fraction organic carbon value should be measured if possible by collecting a sample of aquifer material from an uncontaminated zone and performing a laboratory analysis (e.g. ASTM Method 2974-87 or equivalent). If unknown, a default value of 0.001 is often used (e.g., ASTM 1995).		
How to Enter Data	Enter directly. If the retardation factor is entered directly, this parameter is not needed in BIOSCREEN.		

4. BIODEGRADATION DATA

Parameter	First-Order Decay Coefficient (lambda)
Units	1/yr
Description	Rate coefficient describing first-order decay process for dissolved constituents. The first-order decay coefficient equals 0.693 divided by the half-life of the contaminant in groundwater. In BIOSCREEN, the first-order decay process assumes that the rate of biodegradation depends only on the concentration of the contaminant and the rate coefficient. For example, consider 3 mg/L benzene dissolved in water in a beaker. If the half-life of the benzene in the beaker is 728 days, then the concentration of benzene 728 days from now will be 1.5 mg/L (ignoring volatilization and other losses).
	Considerable care must be exercised in the selection of a first-order decay coefficient for each constituent in order to avoid significantly over-predicting or under-predicting actual decay rates. Note that the amount of degradation that occurs is related to the time the contaminants spend in the aquifer, and that this parameter is not related to the time it takes for the source concentrations to decay by half.
Typical Values	0.1 to 36 yr^{-1} (see half-life values)
Source of Data	Optional methods for selection of appropriate decay coefficients are as follows:
	Literature Values: Various published references are available listing decay half-life values for hydrolysis and biodegradation (e.g., see Howard *et al.*, 1991). Note that many references report the half-lives; these values can be converted to the first-order decay coefficients using $k = 0.693 / t_{1/2}$ (see dissolved plume half-life).
	Calibrate to Existing Plume Data: If the plume is in a steady-state or diminishing condition, BIOSCREEN can be used to determine first-order decay coefficients that best match the observed site concentrations. One may adopt a trial-and-error procedure to derive a best-fit decay coefficient for each contaminant. For still-expanding plumes, this steady-state calibration method may over-estimate actual decay-rate coefficients and contribute to an under-estimation of predicted concentration levels.
How to Enter Data	1) Enter directly or 2) Fill in the estimated half-life values as described below and have BIOSCREEN calculate the first-order decay coefficients.

Parameter	Dissolved Plume Solute Half-Life (t_h)
Units	years
Description	Time, in years, for dissolved plume concentrations to decay by one half as contaminants migrate through the aquifer. Note that the amount of degradation that occurs is related to the time the contaminants spend in the aquifer, and that the degradation IS NOT related to the time it takes for the source concentrations to decay by half.
	Modelers using the first-order decay model typically use the first-order decay coefficient as a calibration parameter, and adjust the decay coefficient until the model results match field data. With this approach, uncertainty in a number of parameters (e.g., dispersion, sorption, biodegradation) are lumped together in a single calibration parameter.
	Considerable care must be exercised in the selection of a first-order decay coefficient for each contaminant in order to avoid significantly over-predicting or under-predicting actual decay rates.
Typical Values	Benzene 0.02 to 2.0 yrs Toluene 0.02 to 0.17 yr Ethylbenzene 0.016 to 0.62 yr Xylene 0.038 to 1 yr (from ASTM, 1995)
Source of Data	Optional methods for selection of appropriate decay coefficients are as follows: **Literature Values:** Various published references are available listing decay half-life values for hydrolysis and biodegradation (e.g., see Howard et al. 1991). **Calibrate to Existing Plume Data:** If the plume is in a steady-state or diminishing condition, BIOSCREEN can be used to determine first-order decay coefficients that best match the observed site concentrations. A trial-and-error procedure may be adopted to derive a best-fit decay coefficient for each contaminant. For expanding plumes, this steady-state calibration method may over-estimate actual decay-rate coefficients and contribute to an under-estimation of predicted concentration levels.
How to Enter Data	Enter directly. If the first-order decay coefficient is entered directly, this parameter is not needed in BIOSCREEN

Parameter	Delta Oxygen (O₂)
Units	mg/L
Description	This parameter, used in the instantaneous reaction model, is one component of the total biodegradation capacity of the groundwater as it flows through the source zone and contaminant plume. The model assumes that 3.14 mg of oxygen are required to consume 1 mg of BTEX (Wiedemeier, Wilson, et al., 1995). Note that this parameter is used for the instantaneous reaction model, which is appropriate only for readily biodegradable compounds such as BTEX that degrade according to the assumed BIOSCREEN utilization factors, and is not appropriate for more recalcitrant compounds such as the chlorinated solvents.
Typical Values	Data from 28 AFCEE sites (see Table 1): Median = 5.8 mg/L Maximum = 12.7 mg/L Minimum = 0.4 mg/L.
Source of Data	For planning studies, typical values taken from Table 1 can be used. For actual RNA studies, the Air Force Intrinsic Remediation Technical Protocol (Wiedemeier, Wilson, et al., 1995) should be applied. Enter the average background concentration of oxygen minus the lowest observed concentration of oxygen in the source area. BIOSCREEN automatically applies the utilization factor used to compute a biodegradation capacity.
How to Enter Data	Enter directly.

Parameter	Delta Nitrate (NO₃)
Units	mg/L
Description	This parameter, used in the instantaneous reaction model, is one component of the total biodegradation capacity of the groundwater as it flows through the source zone and contaminant plume. The model assumes that 4.9 mg of nitrate are required to consume 1 mg of BTEX (Wiedemeier, Wilson, et al., 1995). Note that this parameter is used for the instantaneous reaction model, which is appropriate only for readily biodegradable compounds such as BTEX that degrade according to the assumed BIOSCREEN utilization factors, and is not appropriate for more recalcitrant compounds such as the chlorinated solvents.
Typical Values	Data from 28 AFCEE sites (see Table 1): Median = 6.3 mg/L Maximum = 69.7 mg/L Minimum = 0 mg/L.
Source of Data	For planning studies, typical values taken from Table 1 can be used. For actual RNA studies, the Air Force Intrinsic Remediation Technical Protocol (Wiedemeier, Wilson, et al., 1995) should be applied. Enter the average background concentration of nitrate minus the lowest observed concentration of nitrate in the source area. BIOSCREEN automatically applies the utilization factor to compute a biodegradation capacity.
How to Enter Data	Enter directly.

Parameter	Observed Ferrous Iron (Fe^{2+})
Units	mg/L
Description	This parameter, used in the instantaneous reaction model, is one component of the total biodegradation capacity of the groundwater as it flows through the source zone and contaminant plume. Ferrous iron is a metabolic by-product of the anaerobic reaction where solid ferric iron is used as an electron acceptor. The model assumes that 21.8 mg of ferrous iron represents the consumption of 1 mg of BTEX (Wiedemeier, Wilson, et al., 1995). Note that this parameter is used for the instantaneous reaction model, which is appropriate only for readily biodegradable compounds such as BTEX that degrade according to the assumed BIOSCREEN utilization factors, and is not appropriate for more recalcitrant compounds such as the chlorinated solvents. Some researchers suggest the observed ferrous iron concentration is much less (10% or less) than the actual amount of ferrous iron that has been generated due to the sorption of ferrous iron onto the aquifer matrix (Lovely, 1995). If this is the case, then the value used for this parameter should be much higher than the observed maximum concentration of ferrous iron in the aquifer.
Typical Values	Data from 28 AFCEE sites (see Table 1): Median = 16.6 mg/L. Maximum = 599.5 mg/L. Minimum = 0 mg/L
Source of Data	For planning studies, typical values taken from Table 1 can be used. For actual RNA studies, the Air Force Intrinsic Remediation Technical Protocol (Wiedemeier, Wilson, et al., 1995) should be applied. Enter the average observed concentration, in mg/L, of ferrous (dissolved) iron found in the source area (approximately the area where ferrous iron has been observed in monitoring wells). BIOSCREEN automatically applies the utilization factor to compute a biodegradation capacity.
How to Enter Data	Enter directly.

Parameter	Delta Sulfate (SO₄)
Units	mg/L
Description	This parameter, used in the instantaneous reaction model, is one component of the total biodegradation capacity of the groundwater as it flows through the source zone and contaminant plume. The model assumes that 4.7 mg of sulfate are required to consume 1 mg of BTEX (Wiedemeier, Wilson, *et al.*, 1995). Note that this parameter is used for the instantaneous reaction model, which is appropriate only for readily biodegradable compounds such as BTEX that degrade according to the assumed BIOSCREEN utilization factors, and is not appropriate for more recalcitrant compounds such as the chlorinated solvents.
Typical Values	Data from 28 AFCEE sites (see Table 1): Median = 24.6 mg/L · Maximum = 109.2 mg/L Minimum = 0 mg/L
Source of Data	For planning studies, typical values taken from Table 1 can be used. For actual RNA studies, the Air Force Intrinsic Remediation Technical Protocol (Wiedemeier, Wilson, *et al.*, 1995) should be applied. Enter the average background concentration of sulfate minus the lowest observed concentration of sulfate in the source area. BIOSCREEN then computes a biodegradation capacity.
How to Enter Data	Enter directly.
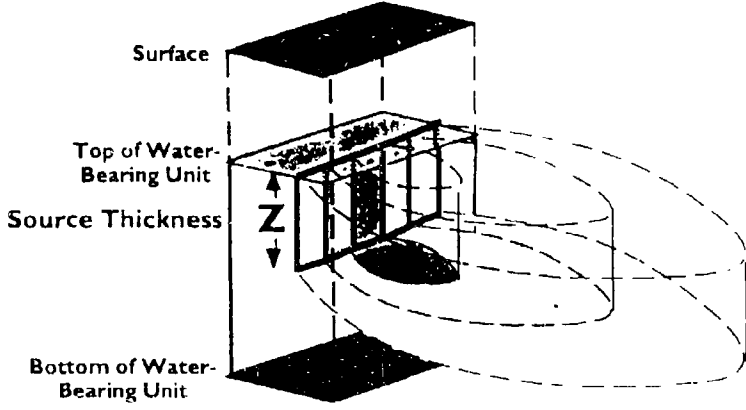
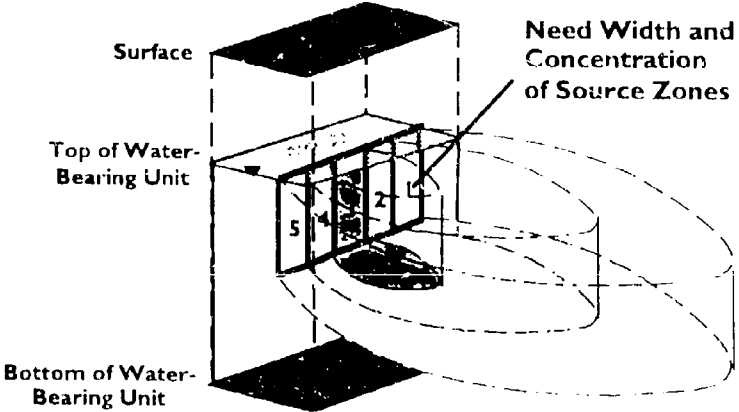| Parameter	Observed Methane (CH₄)
Units	mg/L
Description	This parameter, used in the instantaneous reaction model, is one component of the total biodegradation capacity of the groundwater as it flows through the source zone and contaminant plume. Methane is a metabolic by-product of methanogenic activity. The model assumes that 0.78 mg of methane represents the consumption of 1 mg of BTEX (Wiedemeier, Wilson, *et al.*, 1995). Note that this parameter is used for the instantaneous reaction model, which is appropriate only for readily biodegradable compounds such as BTEX that degrade according to the assumed BIOSCREEN utilization factors, and is not appropriate for more recalcitrant compounds such as the chlorinated solvents.
Typical Values	Data from 28 AFCEE sites (see Table 1): Median = 7.2 mg/L Maximum = 48.4 mg/L Minimum = 0.0 mg/L.
Source of Data	For planning studies, typical values taken from Table 1 can be used. For actual RNA studies, the Air Force Intrinsic Remediation Technical Protocol (Wiedemeier, Wilson, *et al.*, 1995) should be applied. Enter the average observed concentration of methane found in the source area (approximately the area where methane is observed in monitoring wells). BIOSCREEN automatically computes a biodegradation capacity.
How to Enter Data	Enter directly.

5. GENERAL DATA

Parameter	Model Area Length and Width (L and W)
Units	ft
Description	Physical dimensions (in feet) of the rectangular area to be modeled. To determine contaminant concentrations at a particular point along the centerline of the plume (a common approach for most risk assessments), enter this distance in the "Modeled Area Length" box and see the results by clicking on the "Run Centerline" button.
	If one is interested in more accurate mass calculations, make sure most of the plume is within the zone delineated by the Modeled Area Length and Width. Find the mass balance results using the "Run Array" button.
Typical Values	10 to 1000 ft
Source of Data	Values should be slightly larger than the final plume dimensions or should extend to the downgradient point of concern (e.g., point of exposure). If only the centerline output is used, the plume width parameter has no effect on the results.
How to Enter Data	Enter directly.
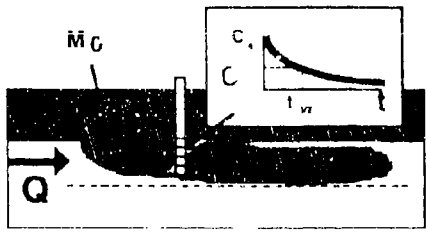
Parameter	Simulation Time (t)
Units	years
Description	Time (in years) for which concentrations are to be calculated. For steady-state simulations, enter a large value (i.e., 1000 years would be sufficient for most sites).
Typical Values	1 to 1000 years
Source of Data	To match an existing plume, estimate the time between the original release and the date the field data were collected. To predict the maximum extent of plume migration, increase the simulation time until the plume no longer increases in length.
How to Enter Data	Enter directly.

6. SOURCE DATA
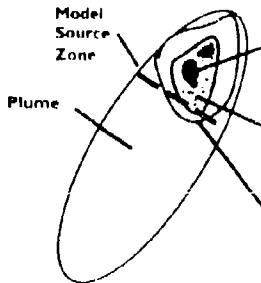
Parameter	Source Thickness In Saturated Zone (z)
Units	ft
Description	The Domenico (1987) model assumes a vertical plane source of constant concentration. For many fuel spill sites the thickness of this source zone is only 5 - 20 ft, as petroleum fuels are LNAPLs (light non-aqueous phase liquids) that float on the water table. Therefore, the residual source zones that are slowly dissolving, creating the dissolved BTEX plume, are typically restricted to the upper part of the aquifer.
Typical Values	5-50 ft
Source of Data	This value is usually determined by evaluating groundwater data from wells near the source zone screened at different depths. If this type of information is not available, then one could estimate the amount of water table fluctuation that has occurred since the time of the release and use this value as the source zone thickness (equating to the smear zone). Otherwise, a simple assumption of 10 feet would probably be appropriate for many petroleum release sites. Note that if DNAPLs are present at the site (e.g., a chlorinated solvent site), a larger source zone thickness would probably be required.
How to Enter Data	Enter directly.

Parameter	Source Zone Width
Units	ft
Description	The Domenico (1987) model assumes a vertical plane source of constant concentration. BIOSCREEN expands the simple one source-zone approach by allowing up to five source zones with different concentrations to account for spatial variations in the source area.
Typical Values	10 - 200 ft
Source of Data	To define a varying source concentration across the site: 1) Draw a line perpendicular to the groundwater flow direction in the source zone. The source zone is typically defined as being the area with contaminated soils having high concentrations of sorbed organics, free-phase NAPLs, or residual NAPLs. If the source zone covers a large area, it is best to choose the most downgradient or widest point in the source area to draw the perpendicular-to-flow line. 2) Divide the line into 1, 3, or 5 zones. A total of 5 zones is shown on the input screen. 3) Determine the width and corresponding average concentration of Zones 1, 2, and 3. Typically Zone 3 will contain the highest concentration. Note that the model assumes the source zone is symmetrical and will automatically define source zones 4 and 5 to be identical to Zones 2 and 1. Therefore, it is not necessary to specify all 5 zones. For simpler problems, you can either use three zones to define varying source concentrations across the site (enter information in Zones 2 and 3, and the model will define Zone 4) or just use a single zone (enter data for Zone 3 only). 4) Enter the width and source concentration into the appropriate zones on the spreadsheet. For example, if a total source width of 100 ft. is divided into five zones, enter 20 ft for each zone width. Enter the average concentration observed across each zone.
How to Enter Data	Enter directly.

Parameter	Source Zone Concentration
Units	mg/L
Description	BIOSCREEN requires source zone concentrations that correspond to the source zone width data (see previous page). Suggested rules of thumb regarding how to handle multiple constituents are: 1) If the maximum plume length is desired, model **lumped constituents** (such as BTEX). If a risk assessment is being performed, data on **individual constituents** are needed. 2) If **lumped constituents** are being modeled (BTEX all together), use either average values for the chemical-specific data (Koc and lambda) or the worst-case values (e.g., use the lowest of the Koc and lambda from the group of constituents being modeled) to overestimate concentrations. Most modeling will be performed assuming that the ratio of BTEX at the edge of the plume is the same as at the source. For more detailed modeling studies, Wilson (1996) has proposed the following rules o help account for different rates of reaction among the BTEX compounds: • If the site is dominated by **aerobic degradation** (most of the biodegradation capacity is from oxygen, a relatively rare occurrence) assume that the benzene will degrade first and that the dissolved material at the edge of the plume is primarily TEX. • If the site is dominated by **nitrate utilization** (most of the biodegradation capacity is from nitrate, a relatively rare occurrence) assume that benzene will degrade last and that the dissolved material at the edge of the plume is primarily benzene. • If the site is dominated by **sulfate reduction** (most of the biodegradation capacity is due to sulfate utilization, a more common occurrence) assume that the benzene will degrade at the same rate as the TEX constituents and that the dissolved material at the edge of the plume is a mixture of BTEX. • If the site is dominated by **methane production** (most of the biodegradation capacity is due to methanogenesis, a more common occurrence) assume that benzene will degrade last and that the dissolved material at the edge of the plume is primarily benzene. 3) If **individual constituents** are being modeled with the instantaneous reaction assumption, note that the total biodegradation capacity must be reduced to account for electron acceptor utilization by other constituents present in the plume. For example, in order to model benzene as an individual constituent using the instantaneous reaction model in a BTEX plume containing equal source concentrations of benzene, toluene, ethylbenzene and xylene, the amount of oxygen, nitrate, sulfate, iron, and methane should be reduced by 75% to account for utilization by toluene, ethylbenzene, and xylene.
Typical Values	0.010 to 120 mg/L.
Source of Data	Source area monitoring well data (see figure on previous page).
How to Enter Data	Enter directly.

Parameter	Source Half-Life (Value Calculated by Model)
Units	years
Description	The Domenico (1987) model assumes the source is infinite, i.e. the source concentrations are constant. In BIOSCREEN, however, an approximation for a declining source concentration has been added. Note that this is an experimental relationship, and it should be applied with caution. The declining source term is based on the following assumptions:

* There is a finite mass of organics in the source zone present as a free-phase or residual NAPL. The NAPL in the source zone dissolves slowly as fresh groundwater passes through.

* The change in source zone concentration can be approximated as a first-order decay process. For example, if the source zone concentration "half-life" is 10 years and the initial source zone concentration is 1 mg/L, then the source zone concentration will be 0.5 mg/L after 10 years, and 0.25 mg/L after 20 years.

Note that the assumption that dissolution is a first-order process is only an approximation, and that source attenuation is best described by first-order decay when concentrations are relatively low (< 1 mg/L). For more information on dissolution, see Newell et al., (1994). The source half-life IS NOT related to lambda, the biodegradation half-life for dissolved constituents. Lambda is used to calculate the amount of biodegradation of dissolved organics after they leave the source zone and travel through the plume area. The source half-life is related to the rate of dissolution occurring in the source zone, and describes the change in source concentrations over time.

* The BIOSCREEN software automatically calculates the source zone concentration half-life if the user enters a best estimate for the mass of dissolvable organics zone (soluble organic constituents sorbed on the soil, residual NAPLs, and free product) in the source. The half-life of the dissolution process can be approximated if one knows the mass of dissolvable organics in the source zone (in mg or kg), the flow rate through the source zone, and the average concentration of dissolved organics that leave the source zone. The equation is based on integrating the concentration vs. time relationship (first-order decay) and using the relationship that the mass in the source zone over time is proportional to the source concentration over time. This yields the following expression for the half-life of the concentration of dissolved organics in the source zone (see Appendix A.3):

$$t_{half\ source} = (0.693 * M_0)/(Q * C_0) \quad where$$

$t_{half\ source}$ = Half life of source concentration (yrs)

Q = Groundwater flow through source zone (L/yr)

C_0 = Effective source zone conc. (observed concentration + biodeg. capacity for inst. react. assumption) at t = 0 (mg/L)

M_0 = Mass of dissolvable organics in source zone at t = 0 (mg)

Parameter	Source Half-Life (Value Calculated by Model) (Cont'd)
Description (cont'd) **Key Questions:**	Why are there two source half-lives reported? Note that BIOSCREEN automatically selects the correct source half-life value depending on which kinetic model is being used (see Which Model Should One Use? under BIOSCREEN Concepts). Two source half-lives are reported by the model in the source half-life cell: the smaller number will be the source half-life from dissolution if Instantaneous Reaction kinetics are used, and the larger value will be for No Degradation or First-order Decay kinetics. The first-order decay model assumes biodegradation starts immediately downgradient of the source, and that the rate of dissolution is reflected by the concentration of dissolved organics actually measured in monitoring wells. In other words, the first-order decay model assumes C_0 is equal to the observed source concentration. The instantaneous reaction model assumes biodegradation is occurring directly in the source zone, and that the **effective** source zone concentration C_0 is equal to the measured concentration in the source zone plus any "missing" concentration due to biodegradation. For example, if the source zone concentration in monitoring wells is 5 mg/L, and the biodegradation capacity is 10 mg/L, the effective source concentration C_0 ncentration before biodegradation) is 15 mg/L. In other words, C_0 is equal to the measured source concentration plus the biodegradation capacity provided by the electron acceptor concentration. This means use of the instantaneous reaction assumption will result in higher dissolution rates and shorter source lifetimes (see Newell et al., 1995). **Does BIOSCREEN account for travel time away from the declining source?** With the declining source option in BIOSCREEN, the concentration for any location and any time is calculated using a source concentration determined by the first-order decay calculations shown above. The time used to determine the source concentration is adjusted to account for the travel time between the source and measurement point. For example, consider the case where a declining source term is used with a source half-life of 10 years and a solute velocity of 100 ft/yr. To calculate the concentration at a point 2000 ft away at time 30 years, BIOSCREEN follows these steps. 1) Calculates travel time from point to source: 2000/100 20 years 2) Subtracts travel time from simulation time: 30 yrs - 20 yrs = 10 yrs 3) Calculates source decay coeff.: ksource = 0.693/(source half life) 4) Calculates source conc. at t = 10 yr: $C_{10} = C_0 \exp$
Typical Values	1 to 10,000 years
Source of Data	Calculated by model from soluble mass in NAPL and soil (see below), source concentrations, and groundwater velocity.
How to Enter Data	Calculated directly by model. Change by changing soluble mass.

Parameter	Soluble Mass in NAPL Soil
Units	kg
Description	The best estimate of dissolvable organics in the source zone is obtained by adding the mass of dissolvable organics on soils, free-phase NAPLs, and residual NAPLs. This quantity is used to estimate the rate that the source zone concentration declines. Note that this is an experimental and unverified model that should be applied with care (the model probably underpredicts removal rate).
	For gasoline or JP-4 spills, BTEX is usually assumed to comprise the bulk of dissolvable organics in the source zone. To simulate a declining source, use the method described below. For constant-source simulations, either enter a very large number for soluble mass in the source zone (e.g., 1,000,000 kg) or type "Infinite".
Typical Values	0.1 to 100,000 kg
Source of Data	This information will most likely come from either:
	1) Estimates of the mass of spilled fuel (remember to convert the total mass of spilled fuel to the dissolvable mass; for example BTEX represents only 5-15% of the total mass of gasoline).
	2) Integration of maps showing contaminated soil zones (data in mg/kg) and/or NAPL zones (usually product thickness). The user should estimate the volume of contaminated soil, convert to kg of contaminated soil, and multiply by the average soil concentration. To make the estimate more accurate, the user might have to divide the soil into different zones of soil concentrations, into unsaturated vs. saturated soil, and/or into different depths. (One standard approach is to divide into a vertically averaged unsaturated zone map and a vertically averaged saturated zone map.) If the user is making estimates from NAPL data, remember the thickness of product in a aquifer is only 10-50% of the actual product thickness in the well (Bedient et al., 1994)
	Note that the data is to be entered in kg, and the model will convert the results to estimate the source half-life. An example is provided below assuming a bulk density of 1.7 kg/L (e.g., 100 ft² x 20 ft x 28.3 L/ft³ x 1.7 kg/L x 600 mg/Kg x 10⁻⁶ kg/mg = 58 kg):
How to Enter Data	Enter directly

7. FIELD DATA FOR COMPARISON

Parameter	Field Data for Comparison
Units	mg/L
Description	These parameters are concentrations of dissolved organics in wells near the centerline of the plume. These data are used to help calibrate the model and are displayed with model results in the "Run Centerline" option.
Typical Values	0.001 to 50 mg/L
Source of Data	Monitoring wells located near the centerline of the plume.
How to Enter Data	Enter as many or as few of these points as needed. The data are used only to help calibrate the model when comparing the results from the centerline option. Note that the distance from source values cannot be changed; use the closest value possible.

ANALYZING BIOSCREEN OUTPUT

The output shows concentrations along the centerline (for all three kinetic models at the same time) or as an array (one kinetic model at a time). Note that the results are all for the time entered in the "Simulation Time" box.

Centerline Output

Centerline output is displayed when the "Run Centerline" button is pressed on the input screen. The centerline output screen shows the average concentration at the top of the saturated zone (Z=0) along the centerline of the plume (Y=0). Clicking on "Animate" divides the simulation into 10 separate time periods and shows the movement of the plume based on the three BIOSCREEN models (red: no degradation, blue: first-order decay, green: instantaneous reaction). Note that all concentrations are displayed in units of mg/L.

Array Output

The array output is displayed when the "Run Array" button is pressed on the input screen. The user is asked to select one of the three model types (no degradation, first-order decay, or instantaneous reaction). A 3-D graphic shows results on a 10-point long by 5-point-wide grid. To alter the modeled area, adjust the Model Area Length and Width parameters on the input screen.

To see the plume array that exceeds a certain target level (such as an MCL or risk-based cleanup level), enter the target level in the box and push "Plot Data > Target". Only sections of the plume exceeding the target level will be displayed. To see all the data again, push "Plot All Data". Note that BIOSCREEN automatically resets this button to "Plot All Data" when the "Run Array" button is pressed on the input screen. An approximate mass balance is presented on the array output screen as described below.

Calculating the Mass Balance

Plume Mass if No Biodegradation(kg)

The model calculates the total amount of dissolved contaminant that has left the source zone. If the source is an infinite source, then the calculation is based on the discharge of groundwater through the source zone (Darcy velocity for groundwater times the total source width times the source depth) times the average concentration of the source zone (a weighted average of concentration and source length for each of the different source zones) times the simulation time.

If the source is a declining source, an exponential source decay term is used to estimate the mass of organics that have left the source zone (see Source Data: Varying Concentrations Over Time). Note that the source decay term is for dissolution of soluble organics from the source zone and is not related to the first-order decay term for the dissolved constituents.

Note that the total mass in the plume is the same for the No Degradation and First-order Decay models but is different for the Instantaneous Reaction model. The source zone dissolution rate is calculated to be much higher if the instantaneous reaction model is selected. The instantaneous reaction assumes that active biodegradation reactions occur in the source zone, and that the observed concentrations of organics in source zone monitoring wells reflect conditions after biodegradation. In this case, the actual concentration of organics coming off the source zone is equal to the measured concentration plus the biodegradation capacity of the upgradient groundwater. The resulting higher effective dissolution rate equates to a greater amount of mass leaving the source area, leading to different mass values for the Instantaneous Reaction model.

Actual Plume Mass(kg)

BIOSCREEN calculates the mass of organics in the 5x10 plume array for the three models:

1) No Degradation   2) 1st Order Decay   3) Instantaneous Reaction

The mass is calculated by assuming that each point represents a cell equal to the incremental width and length (except for the first column which is assumed to be half as long as the other columns because the source is assumed to be in the middle of the cell). The volume of affected groundwater in each cell is calculated by multiplying the area of each cell by the source depth and by porosity (the mass balance calculation assumes 2-D transport). The mass of organics in each cell is then determined by multiplying the volume of groundwater by the concentration and then by the retardation factor (to account for sorbed constituents).

How BIOSCREEN Estimates Actual Plume Mass for Biodegradation Models

If the mass of organics in the 5x10 plume array is within 50% to 150% of the mass of organics that have left the source (see box above), then two values are calculated:

% Biodegraded, 1st order decay = (Plume Mass, 1st order decay) * 100 / (Plume mass, no biodeg)

% Biodegraded, inst. react. = (Plume Mass, inst. react) * 100 / (Plume mass, no biodeg)

These percentages are multiplied against the Plume Mass if No Biodegradation Value (first box) to estimate the actual plume mass for the two biodegradation models. If the No Degradation model has been selected, there is no biodegradation, and the Actual Plume Mass (second box) will equal the Plume Mass if No Biodegradation (first box).

If BIOSCREEN Says "Can't Calc"

If the mass of organics in the plume does not fall within 50% to 150% of the mass of organics that have left the source (first box), then the model concludes that the modeled area (see Input Screen, Section 5: General Data) is not sized correctly to capture enough mass in the 5X10 array and writes "Can't Calc" in the box. The user is encouraged to adjust the modeled length and width to capture most of the No Degradation plume in the 5x10 array. In addition, sometimes source conditions with variable concentrations and widths (see input screens) can make it difficult to accurately capture the plume mass. If the user has problems obtaining a mass balance even after changing the modeled area, change the source term to a single source zone (instead of 3 or 5 zones) to improve the accuracy of the mass balance.

If problems still exist, ensure that the vertical dispersivity term (Section 2 on the Input Screen) is set to 0 (the default value). The mass balance calculations are less accurate for three-dimensional simulations.

Plume Mass Removed by Biodegradation (kg)

An estimate of the mass of contaminants that are biodegraded is provided in BIOSCREEN. The model subtracts the Actual Plume Mass (second box) from the Plume Mass if No Biodegradation (first box). For the No Degradation model, the first box equals the second box, and **Plume Mass Removed by Biodeg** is zero. For the other two cases, the 2 boxes will differ, and the amount of biodegradation will be calculated. The value beneath the third box shows the % of organics that have left the source and have been biodegraded.

Change in Electron Acceptor/Byproduct Masses (kg)

BIOSCREEN uses the Plume Mass Removed by Biodegradation to back-calculate the amount of measurable electron acceptors consumed and the amount of measurable metabolic by-products that have been produced.

For example, the amount of oxygen consumed is calculated by:

Oxygen Consumed (kg) = **(Plume Mass Removed by Biodeg)** * (Delta O2/Util. Fact.)

$$(\text{Biodeg. Capacity})$$

(see Biodegradation Capacity section to see how this term is calculated)

Note that the total sum of consumed electron acceptors does not equal the Plume Mass Removed by Biodegradation. This is because the stoichiometry of the biodegradation reactions do not represent a 1:1 relationship between the mass of hydrocarbon and electron acceptor consumed (see Utilization Factor section).

Original Mass in Source (kg)

Equal to the Soluble Mass in NAPL and Soil entered by the user on the Input Screen. If the user has selected an "Infinite" mass to simulate a non-declining source, this box will show "Infinite."

Mass in Source Now (kg)

The amount of mass remaining in the source zone at the end of the simulation period is calculated and displayed in this box. This calculation is performed as follows:

(Mass in the Source Now) =

(Original Mass in Source) - (Actual Plume Mass + Plume Mass Removed by Biodeg)

Current Volume of Groundwater in Plume (ac-ft)

If the mass of organics in the plume falls within 50% to 150% of the mass of organics that have left the source (first box), then the model concludes the modeled area (see Input Screen, Section 5: General Data) is appropriately sized to estimate the volume of the plume. In this case BIOSCREEN counts the number of cells in the 5 x 10 array with concentration values greater than 0, and multiplies this by the volume of groundwater in each cell (length * width * source thickness * porosity).

If the user wishes to estimate the volume of the plume above a certain target level, enter the target level in the appropriate box and press the appropriate model to display the result (No Degradation, 1st Order Decay, or Instantaneous Reaction).

Note that the model does not account for the effects of any vertical dispersion.

Flowrate of Water Through Source Zone (ac-ft/yr)

Using the Darcy velocity, the source thickness, and the source width, BIOSCREEN calculates the rate that clean groundwater moves through the source zone where it will pick up dissolved hydrocarbons. Note that the groundwater Darcy velocity is equal to the groundwater seepage velocity multiplied by porosity.

BIOSCREEN TROUBLESHOOTING TIPS

Minimum System Requirements

The BIOSCREEN model requires a computer system capable of running Microsoft® Excel 5.0 for Windows. Because of the volume of calculations required to process the numerical data generated by the model, GSI recommends running the model on a system equipped with a 486 DX or higher processor running at 66 MHz or faster. A minimum of 8 Megabytes of system memory (RAM) is strongly recommended.

The model's input and output screens are optimized for display at a monitor resolution of 640x480 (Standard VGA). If you are using a higher resolution, for example 800x600 or 1024x768, see Changing the Model's Display.

For best results, Start Excel and Load the BSCREEN.XLS file from the **File / Open** menu.

Spreadsheet-Related Problems

The buttons won't work: BIOSCREEN is built in the Excel spreadsheet environment, and to enter data one must click anywhere outside the cell where you just entered data. If you can see the numbers you just entered in the data entry part of Excel above the spreadsheet, the data has not yet been entered. Click on another cell to enter the data.

is displayed in a number box: The cell format is not compatible with the value, (e.g. the number is too big to fit into the window). To fix this, select the cell, pull down the format menu, select "Cells" and click on the "Number" tab. Change the format of the cell until the value is visible. If the values still cannot be read, select the format menu, select "Cells" and click on the "Font" tab. Reduce the font size until the value can be read.

#DIV/0! is displayed in a number box: The most common cause of this problem is that some input data are missing. In some cases, entering a zero in a box will cause this problem. Double check to make certain that all of the input cells required for your run have data. Note that for vertical dispersivity, BIOSCREEN will convert a "0" into the data entry cell into a very low number ($1x10^{-99}$) to avoid #DIV/0! errors.

There once were formulas in some of the boxes on the input screen, but they were accidentally overwritten: Click on the "Restore Formulas for Vs, Dispersivities, R, and lambda" button on the bottom right-hand side of the input screen. Note that this button will also restore the formulas that make the Source Width and Source Concentrations for source zones 4 and 5 equal to source zones 2 and 1, respectively.

The graphs seem to move around and change size: This is a feature of Excel. When graph scales are altered to accommodate different plotted data, the physical size of the graphs will change slightly, sometimes resulting in a graph that spreads out over the fixed axis legends. You can manually resize the graph to make it look nice again by double-clicking on the graph and resizing it (refer to the Excel User's Manual).

Common Error Messages

Unable to Load Help File: The most common error message encountered with BIOSCREEN is the message "Unable to Open Help File" after clicking on a Help button. Depending on the version of Windows you are using, you may get an Excel Dialog Box, a Windows Dialog Box, or

you may see Windows Help load and display the error. This problem is rela 'd to the ease with which the Windows Help Engine can find the datafile, BIOSCRN.HLP. Here are some suggestions (in decreasing order of preference) for helping WinHelp find it:

- If you are fortunate enough to be asked to find the requested datafile, do so. It's called BIOSCRN.HLP, and it was installed in the same directory/folder as the BIOSCRN.XLS file.

- Use the File/Open menus from within Excel instead of double-clicking on the filename or Program Manager icon to open the BIOSCRN.XLS file. This sets the "current directory" to the directory containing the Excel file you just opened.

- Change the WinHelp call in the VB Module to "hard code" the directory information. That way, the file name and its full path will be explicitly passed to WinHelp. Hints for doing this are in the VBA module. Select the Macro Module tab and search for the text "Helpfile".

- As a last resort, you can add the BIOSCREEN directory to your path (located in your AUTOEXEC.BAT file), and this problem will be cured. You will have to reboot your machine, however, to make this work

The BIOSCREEN system was designed to be used on a PC with Windows configured to a standard VGA resolution of 640x480 pixels. If you are using a larger monitor and your video resolution is set to 800x600 pixels or greater, you will need to change the zoom factor in the Visual Basic code.

In the first three lines in the Macro Module of the BIOSCREEN spreadsheet, change the number after the equals sign in the following line:

Const ZoomValue = 65

If your display resolution is standard VGA (640x480), use 65 for the zoom value. If your resolution is 800x600, use a zoom value of 82. If your resolution is not 640x480 or 800x600, if your video performance is seriously degraded, or if you experience display problems, you may need to change your video resolution (see the online help for Windows Setup or consult your Windows installation manuals) and experiment with other values for ZoomValue.

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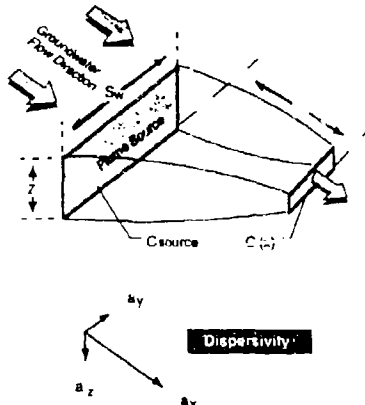
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APPENDIX A.1 DOMENICO ANALYTICAL MODEL

The Domenico (1987) analytical model, used by BIOSCREEN, is designed for the multidimensional transport of a decaying contaminant species. The model equation, boundary conditions, assumptions, and limitations are discussed below.

Domenico Model with Instantaneous Reaction Superposition Algorithm

$$\frac{C(x,y,o,t)}{(Co+BC)} = \frac{1}{8}\exp\left[\frac{x}{\alpha_x 2}\left(1-\left(1+4\lambda\alpha_x/v\right)^{1/2}\right)\right]$$

$$erfc\left[\frac{\left(x-vt\left(1+4\lambda\alpha_x/v\right)^{1/2}\right)}{2(\alpha_x vt)^{1/2}}\right]$$

$$\left\{erf\left[\frac{(y+Y/2)}{2(\alpha_y x)^{1/2}}\right]-erf\left[\frac{(y-Y/2)}{2(\alpha_y x)^{1/2}}\right]\right\}$$

$$\left\{erf\left[\frac{(Z)}{2(\alpha_z x)^{1/2}}\right]-erf\left[\frac{(-Z)}{2(\alpha_z x)^{1/2}}\right]\right\}-B$$

where: $\quad v = \dfrac{K \cdot i}{\theta_e R} \qquad BC = \Sigma\,\dfrac{C(ea)_n}{UF_n}$

Definitions

BC	Biodegradation capacity (mg/l)
C(x,y,z,t)	Concentration at distance x downstream of source and distance y off centerline of plume at time t (mg/L).
C_s	Concentration in Source Zone (mg/L.)
C_0	Concentration in Source Zone at t=0 (mg/L)
x	Distance downgradient of source (ft)
y	Distance from plume centerline of source (ft)
z	Distance from surface to measurement point (assumed to be 0; concentration is always assumed to be at top of water table)
$C(ea)_n$	Concentration of electron acceptor n in groundwater (mg/L)

UF_n	Utilization factor for electron acceptor n (i.e., mass ratio of electron acceptor to hydrocarbon consumed in biodegradation reaction)
α_x	Longitudinal groundwater dispersivity (ft)
α_y	Transverse groundwater dispersivity (ft)
α_z	Vertical groundwater dispersivity (ft)
θ_e	Effective Soil Porosity
λ	First-Order Degradation Rate (day^{-1})
v	Groundwater Seepage Velocity (ft/yr)
K	Hydraulic Conductivity (ft/yr)
R	Constituent retardation factor
i	Hydraulic Gradient (cm/cm)
Y	Source Width (ft)
Z	Source Depth (ft)

The initial conditions are:

1) $c(x, y, z, 0) = 0$ (Initial concentration $= 0$ for x, y, z, > 0)

2) $c(0, Y, Z, 0) = C_0$ (Source concentration for each vertical plane source $= C_0$ at time 0)

The key assumptions in the model are:

1) The aquifer and flow field are homogeneous and isotropic.

2) The groundwater velocity is fast enough that molecular diffusion in the dispersion terms can be ignored (may not be appropriate for simulation of transport through clays).

3) Adsorption is a reversible process represented by a linear isotherm.

The key limitations to the model are:

1)   The model should not be applied where pumping systems create a complicated flow field.

2)   The model should not be applied where vertical flow gradients affect contaminant transport.

3)   The model should not be applied where hydrogeologic conditions change dramatically over the simulation domain

The most important modifications to the original Domenico model are:

1)   The addition of "layer cake" source terms where three Domenico models are superimposed one on top of another to yield the 5-source term used in BIOSCREEN (see Connor et al., 1994; and the Source Width description in the BIOSCREEN Data Entry Section).

2)   Addition of the instantaneous reaction term using the superposition algorithm (see Appendix A.2, below). For the instantaneous reaction assumption, the source concentration is assumed to be an "effective source concentration" (Coe) equal to the observed concentration in the source zone plus the biodegradation capacity (see "Source Concentration" on the BIOSCREEN Data Entry section).

APPENDIX A.2 INSTANTANEOUS REACTION - SUPERPOSITION ALGORITHM

Early biodegradation research focused on the role of dissolved oxygen in controlling the rate of biodegradation in the subsurface (Borden et al., 1986; Lee et al, 1987). Because microbial biodegradation kinetics are relatively fast in comparison to the rate of oxygen transport in the groundwater flow system, Borden demonstrated that the biodegradation process can be simulated as an instantaneous reaction between the organic contaminant and oxygen. This simplifying assumption was incorporated into the BIOPLUME I numerical model which calculated organic mass loss by superposition of background oxygen concentrations onto the organic contaminant plume. In BIOPLUME II, a dual-particle mover procedure was incorporated to more accurately simulate the separate transport of oxygen and organic contaminants within the subsurface (Rifai et al, 1987; Rifai, et al, 1988).

In most analytical modeling applications, contaminant biodegradation is estimated using a first-order decay equation with the biodecay half-life values determined from research literature or site data. However, by ignoring oxygen limitation effects such first-order expressions can significantly overestimate the rate and degree of biodegradation, particularly within low-flow regimes where the rate of oxygen exchange in a groundwater plume is very slow (Rifai, 1994). As a more accurate method of analysis, Newell recommended incorporation of the concept of oxygen superposition into an analytical model (Connor et al., 1994) in a manner similar to that employed in the original BIOPLUME model (Borden et al. 1986). By this method, contaminant mass concentrations at any location and time within the flow field are corrected by subtracting 1 mg/L organic mass for each 3 mg/L of background oxygen, in accordance with the instantaneous reaction assumption. Borden et al (1986) concluded this simple superposition technique was an exact replacement for more sophisticated oxygen-limited models, as long as the oxygen and the hydrocarbon had the same transport rates (e.g., retardation factor, R = 1).

In their original work, Borden et al. (1986) noted that for highly sorptive contaminants the oxygen-superposition method might erroneously characterize biodegradation due to the differing transport rates of dissolved oxygen and the organic contaminant within the aquifer matrix. However, as demonstrated by Connor et al. (1994), the oxygen superposition method and BIOPLUME II (dual particle transport) are in reasonable agreement for contaminant retardation factors as high as 6. Therefore, the superposition method can be employed as a reasonable approximation in BIOSCREEN regardless of contaminant sorption characteristics.

BIOSCREEN employs the same superposition approach for all of the aerobic and anaerobic biodegradation reactions (based on evaluation of O_2, NO_3, SO_4, Fe^{2+}, and CH_4). Based on work reported by Newell et al. (1995), the anaerobic reactions (nitrate, ferric iron, and sulfate reduction and methanogenesis) are amenable to simulation using the instantaneous reaction assumption. The general approach is presented below:
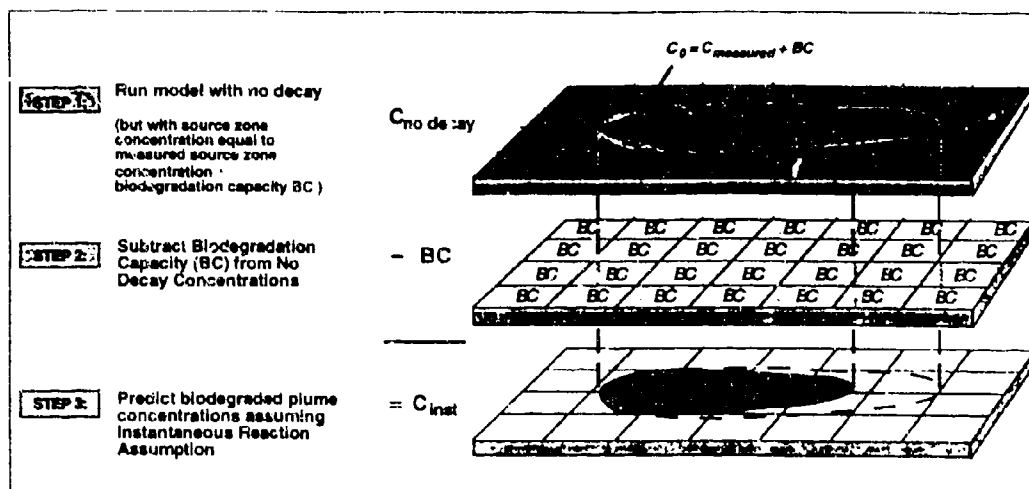
Based on the biodegradation capacity of electron acceptors present in the groundwater system this algorithm will correct the non-decayed groundwater plume concentrations predicted by the Domenico model (Appendix A.1) for the effects of organic constituent biodegradation.

To summarize:

1) The original BIOPLUME model (Borden et al. 1986) used a superposition method to simulate the fast or "instantaneous" reaction of dissolved hydrocarbons with dissolved oxygen in groundwater.

2) Borden et al. (1986) reported that this version of BIOPLUME was mathematically exact for the case where the retardation factor of the contaminant was 1.0.

3) Rifai and Bedient (1990) developed the BIOPLUME II model with a dual-particle tracking routine that expanded the original BIOPLUME model to handle contaminants with retardation factors other than 1.0, in addition to other improvements.

4) Connor et al. (1994) compared the superposition method with the more sophisticated BIOPLUME II model and determined that the two approaches yielded very similar results for readily biodegradable contaminants with retardation factors between 1.0 and 6.0.

5) BIOSCREEN was developed using the superposition approach to simulate the "instantaneous" reaction of aerobic and anaerobic reactions in groundwater. The biodegradation term in BIOSCREEN is mathematically identical to the approach used in the original BIOPLUME model. This mathematical approach (superposition) matches the more sophisticated BIOPLUME II model very closely for readily biodegradable contaminant retardation factors of up to 6.0. BIOSCREEN simulations using the instantaneous reaction assumption at sites with retardation factors greater than 6.0 should be performed with caution and verified using a more sophisticated model such as BIOPLUME III.

APPENDIX A.3 DERIVATION OF SOURCE HALF-LIFE

Purpose: Determine the source half-life relationship used in BIOSCREEN (see Source Half-Life discussion in BIOSCREEN Data Entry Section, pg 30).

Given: 1) There is a finite amount of soluble organic compounds in source zone (the area with contaminated soils and either free-phase or residual NAPL.

2) These organics dissolve slowly as fresh groundwater passes through source zone. Assume the change in mass due to dissolution can be approximated as a first order process:

$$M(t) = M_0 \, e^{-k_s t} \tag{1}$$

Procedure: 1) Calculate initial mass of dissolvable organics in source zone, M_0

2) Determine initial source concentration from monitoring well data, C_0

3) Apply conservation of mass to a control surface containing source zone.

4) Set the expressions for mass at time $t \geq 0$ based on dissolution and conservation of mass equal to each other and solve for an expression describing the concentration at time $t \geq 0$.

5) Apply initial conditions for concentration at time $t=0$ and solve for the first order decay constant, k_s.

Assumptions: 1) Groundwater flowrate is constant, $Q(t)=Q_0$

2) Groundwater flowing through the source zone is free of organic compounds. This implies that no mass is added to the system, only dissolution occurs.

Calculations: 1) Calculate initial mass of dissolved/soluble organic compound, M_0 by using procedure described under "Soluble Mass in NAPL, Soil" page in BIOSCREEN Data Input section.

2) Determine initial concentration, C_0 of organic compound in groundwater leaving the source zone. This may be a spatial average, maximum value, or other value representative of the groundwater concentration leaving the source area. (Note that for the instantaneous reaction assumption, C_0 equals the concentration observed in monitoring wells plus the biodegradation capacity to account for rapid biodegradation reactions in the source zone. See "Soluble Mass in NAPL, Soil" page in BIOSCREEN Data Input section).

$$C(t=0) = C_0 \tag{2}$$

3) Apply conservation of mass to a control surface that contains the source zone. The mass present in the source zone at time $t \geq 0$ is the initial mass plus the change in mass.

$$M(t) \quad M_0 + \iint_{c.s.} \int_t Q(t) \, C(t) \; dt \, dA \tag{3}$$

DERIVATION OF SOURCE HALF-LIFE, Cont'd

Applying the assumptions equation (3) simplifies to

$$M(t)= M_0 - \int_t Q_0\ C(t)\ dt \tag{4}$$

4) Set the two expressions for mass of organic compound in the source zone at time $t \geq 0$ (equations (1) and (4)) equal to each other and solve for an expression describing the concentration leaving the source zone.

$$M_0\ e^{-k_s t} = M_0 - \int_t Q_0\ C(t)\ dt \tag{5}$$

$$\frac{d}{dt}\left[\int_t Q_0 C(t) dt = M_0 - M_0 e^{-k_s t} \right] \tag{6}$$

$$Q_0\ C(t) = k_s\ M_0\ e^{-k_s t} \tag{7}$$

$$C(t) = \frac{k_s M_0}{Q_0} e^{-k_s t} \tag{8}$$

5) Apply the initial condition for concentration leaving the source zone at time $t=0$, eqn (2) to the expression for $C(t)$, eqn (8) and solve for the first order decay coefficient, k_s

$$C_0 = \frac{k_s M_0}{Q_0} \tag{9}$$

$$\therefore \qquad k_s = \frac{Q_0 C_0}{M_0} \tag{11}$$

Summary: The decay coefficient for the source zone in BIOSCREEN is:

$$k_s = \frac{Q_0 C_0}{M_0}$$

The expression for mass at any time $t \geq 0$ is:

$$M(t)= M_0\ e^{-k_s t}$$

Similarly the expression for source zone concentration any time $t \geq 0$ is:

$$C(t)= C_0\ e^{k_s t}$$

APPENDIX A.4 DISPERSIVITY ESTIMATES

Dispersion refers to the process whereby a plume will spread out in a longitudinal direction (along the direction of groundwater flow), transversely (perpendicular to groundwater flow), and vertically downwards due to mechanical mixing in the aquifer and chemical diffusion. Selection of dispersivity values is a difficult process, given the impracticability of measuring dispersion in the field. However, dispersivity data from over 50 sites has been compiled by Gelhar et al. (1992) (see figures A.1 and A.2, next page).

The empirical data indicates that longitudinal dispersivity, in units of length, is related to scale (distance between source and measurement point; the plume length; Lp in BIOSCREEN). Gelhar et al. 1992) indicate there is a considerable range of dispersivity values at any given scale (on the order of 2 - 3 orders of magnitude), 2) suggest using values at the low end of the range of possible dispersivity values, and 3) caution against using a single relationship between scale and dispersivity to estimate dispersivity. However, most modeling studies do start with such simple relationships, and BIOSCREEN is programmed with some commonly used relationships representative of typical and low-end dispersivities:

- **Longitudinal Dispersivity**

$$\text{Alpha x} = 3.28 \; 0.83 \left[\log_{10}\left(\frac{Lp}{3.28} \right) \right]^{2.414} \qquad (Xu \; and \; Eckstein, \; 1995)$$

$$(L_p \; in \; ft)$$

- **Transverse Dispersivity**

Alpha y = 0.10 alpha x   (Based on high reliability

                                            points from Gelhar et al., 1992)

- **Vertical Dispersivity**

Alpha z = very low (i.e. 1 x e-99 ft)   (Based on conservative estimate

Other commonly used relationships include:

Alpha x = 0.1 Lp	(Pickens and Grisak, 1981)
Alpha y 0.33 alpha x	(ASTM, 1995) (EPA, 1986)
Alpha z = 0.05 alpha x	(ASTM, 1995)
Alpha z 0.025 alpha x to 0.1 alpha x	(EPA, 1986)

The BIOSCREEN input screen includes Excel formulas to estimate dispersivities from scale. BIOSCREEN uses the Xu and Eckstein (1995) algorithm for estimating longitudinal dispersivities because 1) it provides lower range estimates of dispersivity, especially for large values of Lp, and 2) it was developed after weighting the reliability of the various field data compiled by Gelhar et al.. (1992) (see Figure A.1). BIOSCREEN also employs low-end estimates for transverse and vertical dispersivity estimates (0.10 alpha x and 0, respectively) because 1) these relationships better fit observed field data reported by Gelhar et al. to have high reliability (see Figure A.2), 2) Gelhar et al. recommend use of values in the lower range of the observed data, and 3) better results were realized when calibrating BIOSCREEN to actual

field sites using lower dispersivities. The user can override these formulas by directly entering dispersivity values in the input screen cell.

Note that the Domenico model and BIOSCREEN are not formulated to simulate the effects of chemical diffusion. Therefore, contaminant transport through very slow hydrogeologic regimes (e.g., clays and slurry walls) should probably not be modeled using BIOSCREEN unless the effects of chemical diffusion are proven to be insignificant. Domenico and Schwartz (1990) indicate that chemical diffusion is small for Peclet numbers (seepage velocity times median pore size divided by the bulk diffusion coefficient) greater than 100.
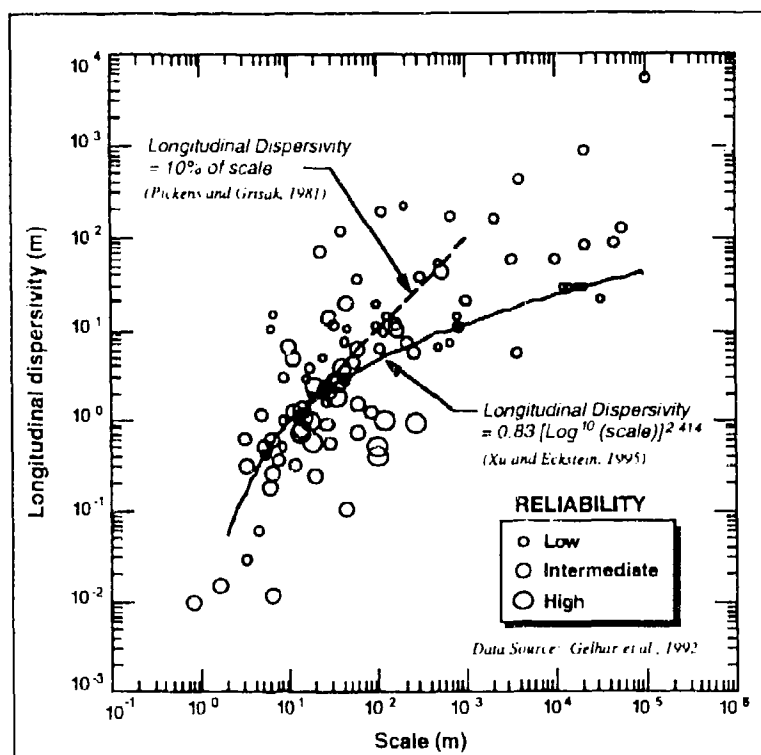
Figure A.1. Longitudinal dispersivity vs. scale data reported by Gelhar et al. (1992). Data includes Gelhar's reanalysis of several dispersivity studies. Size of circle represents general reliability of dispersivity estimates. Location of 10% of scale linear relationship plotted as dashed line (Pickens and Grisak, 1981). Xu and Eckstein's regression (used in BIOSCREEN) shown as solid line. Shaded area defines ± 1 order of magnitude from the Xu and Eckstein regression line and represents general range of acceptable values for dispersivity estimates. Note that BIOSCREEN defines scale as Lp, the plume length or distance to measurement point in ft, and employs the Xu and Eckstein algorithm with a conversion factor (see page 15).
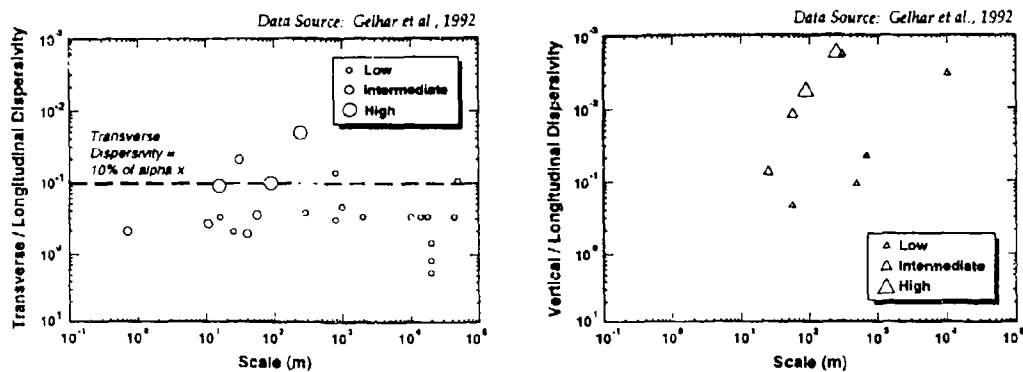
Figure A.2 Ratio of transverse dispersivity and vertical dispersivity to longitudinal dispersivity data vs. scale reported by Gelhar et al. (1992). Data includes Gelhar's reanalysis of several dispersivity studies. Size of symbol represents general reliability of dispersivity estimates. Location of transverse dispersivity relationship used in BIOSCREEN is plotted as dashed line.

APPENDIX A.5 ACKNOWLEDGMENTS

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APPENDIX A.6 BIOSCREEN EXAMPLES

Example 1: SWMU 66, Keesler AFB, Mississippi

- Input Data
- Fig. 1 Source Map
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Example 2: UST Site 870, Hill AFB, Utah

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BIOSCREEN EXAMPLE 1

Keesler Air Force Base, SWMU 66, Mississippi

DATA Type	Parameter	Value	Source of Data
Hydrogeology	• Hydraulic Conductivity: • Hydraulic Gradient: • Porosity:	1.1×10^{-2} (cm/sec) 0.003 (ft/ft) 0.3	• Slug-tests results • Static water level measurements • Estimated
Dispersion	Original: • Longitudinal Dispersivity: • Transverse Dispersivity: • Vertical Dispersivity: After Calibration: • Longitudinal Dispersivity: • Transverse Dispersivity: • Vertical Dispersivity:	 13.3 (ft) 1.3 (ft) 0 (ft) 32.5 (ft) 3.25 (ft) 0 (ft)	• Based on estimated plume length of 280 ft and Xu/Eckstein relationship • Based on calibration to plume length (Note this is well within the observed range for long. dispersivity; see Fig. A.1 in Appendix A..3. Remember to convert from feet to meters before using the chart).
Adsorption	• Retardation Factor: • Soil Bulk Density ρb: • foc: • Koc:	1.0 1.7 (kg/L) 0.0057% B: 38 T: 135 E: 95 X: 240	• Calculated from R = 1+Koc x foc x ρb/n • Estimated • Lab analysis • Literature - use Koc = 38
Biodegradation	Electron Acceptor: Background Conc. (mg/L): Minimum Conc. (mg/L): Change in Conc. (mg/L): Electron Acceptor: Max. Conc. (mg/L): Avg. Conc. (mg/L): Note: Boxed values are BIOSCREEN input values.	O2 NO3 SO4 2.05 0.7 26.2 - 0.4 - 0 - 3.8 1.65 0.7 22.4 Fe CH4 36.1 7.4 16.6 6.6	• Based on March 1995 groundwater sampling program conducted by Groundwater Services, Inc.
General	• Modeled Area Length: • Modeled Area Width: • Simulation Time:	320 (ft) 200 (ft) 6 (yrs)	• Based on area of affected groundwater plume • Steady-state flow
Source Data	• Source Thickness: • Source Concentration:	10 (ft) (See Figure 1)	• Based on geologic logs and lumped BTEX monitoring data
Actual Data	Distance From Source (ft): BTEX Conc. (mg/L):	30 60 180 280 5.0 1.0 0.5 0.001	• Based on observed concentrations at site
OUTPUT	Centerline Concentration:	See Figure 3	
	Array Concentration:	See Figure 4	

Source Zone Assumption

Zone	Width (ft)	Actual Source Conc. In 1995 (mg/L)	Adjusted Model Source Conc. in 1989 (mg/L)
3	14	12	13.7
2	30	2.2	2.5
1	20	0.05	0.06

Note   Source conc. based on Geometric mean between concentration isopleth contours.

SCALE (ft.)
0   40   80

LEGEND

⊙	Monitoring well location
⊛	Temporary cone penetrometer (CPT) piezometer location
0.003	Total BTEX detected in groundwater sample, mg/L
—1.0—	BTEX concentration isopleth, mg/L, March 1995
ND	No BTEX detected
⁝	Affected Soil Zone

BIOSCREEN SOURCE ZONE ASSUMPTIONS

SWMU 66 Site, Keesler AFB, Mississippi

FIGURE 1

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BIOSCREEN Modeling Summary, Keesler Air Force Base, SWMU 66, Mississippi:

- BIOSCREEN was used to try to reproduce the movement of the plume from 1989 (the best guess for when the release occurred) to 1995.

- The soluble mass in soil and NAPL was estimated by integrating BTEX soil concentrations contours mapped as part of the site soil delineation program. An estimated 2000 Kg of BTEX was estimated to be present at the site. This value represented a source half-life of 60 years with the instantaneous reaction model (the first value shown in the source half-life box in Figure 2), a relatively long half-life, so the 2000 Kg measured in 1995 was assumed to be representative of 1989 conditions.

- The instantaneous reaction model was used as the primary model to try to reproduce the plume length (~ 280 ft).

- Because a decaying source was used, the source concentration on the input screen (representing concentrations 6 yrs ago) were adjusted so the source concentration on the centerline output screen (representing concentrations now) were equal to 12 mg/L. Because the source decay term is different for the first order decay and instantaneous reaction models, this simulation focused on matching the instantaneous reaction model. The final result was a source concentration of 13.68 mg/L in the center of the source zone (note on the centerline output the source concentration is 12.021 mg/L).

- The initial run of the instantaneous reaction model indicated that the plume was too long. This indicates that there is more mixing of hydrocarbon and electron acceptors at the site than is predicted by the model. Therefore the longitudinal dispersivity was adjusted upwards (more mixing) until BIOSCREEN matched the observed plume length. The final longitudinal dispersivity was 32.5 ft.

- As a check the first-order decay model was used with the BIOSCREEN default value of 2 yrs. This run greatly overestimated the plume length, so the amount of biodegradation was increased by decreasing the solute half-life. A good match of the plume was reached with a solute half-life of 0.15 years.

- As shown in Figure 3, BIOSCREEN matches the observed plume fairly well. The instantaneous model is more accurate near the source while the first order decay model is more accurate near the middle of the plume. Both models reproduce the actual plume length relatively well.

- As shown in Figure 4, the current plume is estimated to contain 7.8 kg of BTEX. BIOSCREEN indicates that the plume under a no-degradation scenario would contain 126.3 kg BTEX. In other words BIOSCREEN indicates that 94% of the BTEX mass that has left the source since 1989 has biodegraded.

- Most of the source mass postulated to be in place in 1989 is still there in 1996 (2000 kg vs. 1837 kg, or 92% left).

- The current plume contains 1.0 ac-ft of contaminated water, with 1.01^9 acre-ft/yr of water being contaminated as it flows through the source. Because the plume is almost at steady state, 1.019 ac-ft of water become contaminated per year with the same amount being remediated every year due to in-situ biodegradation and other attenuation processes.

Figure 2. BIOSCREEN Input Screen. Keesler Air Force Base, Mississippi.

DISSOLVED HYDROCARBON CONCENTRATION ALONG PLUME CENTERLINE (mg/L at Z=0)

Distance from Source (ft)

TYPE OF MODEL	0	32	64	96	128	160	192	224	256	288	320
No Degradation	13.544	6.575	5.250	4.581	4.107	3.754	3.474	3.241	3.040	2.861	2.697
1st Order Decay	13.544	3.117	1.186	0.488	0.208	0.090	0.040	0.018	0.008	0.004	0.002
Inst. Reaction	12.021	5.463	4.248	3.500	2.860	2.257	1.678	1.114	0.559	0.004	0.000
Field Data from Site	12.000	5.000	1.000				0.500			0.001	
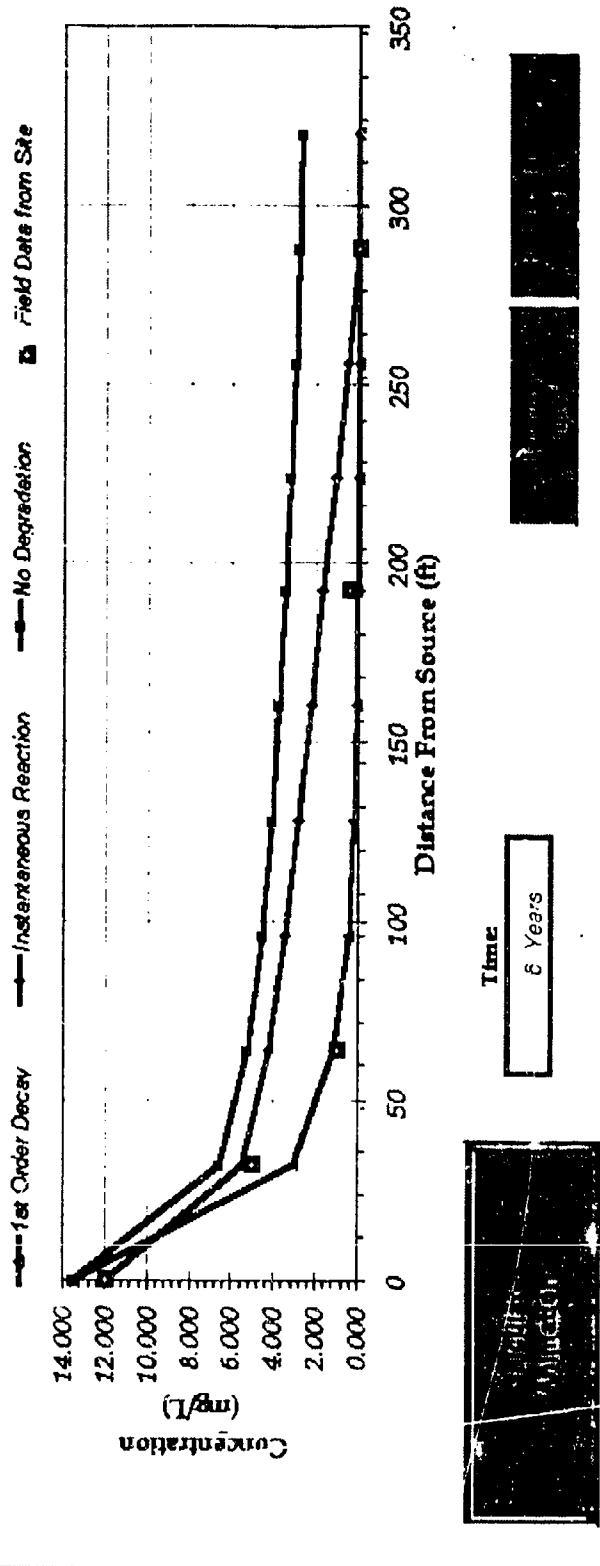
Figure 3. Centerline Output. Keesler Air Force Base, Mississippi.

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DISSOLVED HYDROCARBON CONCENTRATIONS IN PLUME (mg/L at Z=0)

Transverse Distance (ft)

Distance from Source (ft)	0	32	64	96	128	160	192	224	256	288	320
100								0.000	0.000	0.000	0.000
50								0.000	0.000	0.000	0.000
0			4.245				1.678	1.114	1.559	0.004	0.000
-50								0.000	0.000	0.000	0.000
-100								0.000	0.000	0.000	0.000

Time: 6 Years   Target Level: 0.005 mg/L   Displayed Model: Inst. Reaction   Model to Display:

Plume and Source Masses (Order-of-Magnitude Accuracy)

Plume Mass if No Biodegradation: 126.3 (Kg)

- Actual Plume Mass: 7.8 (Kg)

= Plume Mass Removed by Biodeg: 118.6 (Kg) (94 %)

Change in Electron Acceptor/Byproduct Masses:

Oxygen	Nitrate	Iron II	Sulfate	Methane
-13.3	-5.7	+134.3	-181.2	+53.4

Original Mass in Source (Time = 0 Years): 2000.0 (Kg)
Mass in Source Now (Time = 6 Years): 1873.7 (Kg)

Current Volume of Groundwater in Plume: 1.0 (ac-ft)
Flowrate of Water Through Source Zone: 1.019 (ac-ft/yr)
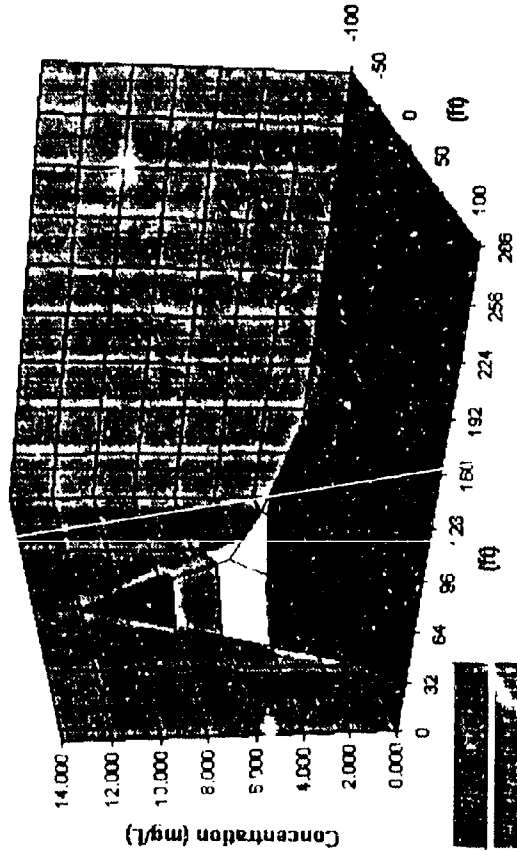
Concentration (mg/L)

Figure 4. Array Concentration Output. Keesler Air Force Base, Mississippi

EXAMPLE 2

Hill Air Force Base, UST Site 870, Utah

DATA TYPE	Parameter	Value	Source
Hydrogeology	• Hydraulic Conductivity: • Hydraulic Gradient: • Porosity:	8.05×10^{-3} (cm/sec) 0.048 (ft/ft) 0.25	• Slug-tests results • Static water level measurements • Estimated
Dispersion	Original • Longitudinal Dispersivity: • Transverse Dispersivity: • Vertical Dispersivity:	28.5 (ft) 2.85 (ft) 0 (ft)	• Based on estimated plume length of 1450 ft and Xu's dispersivity formula • Note: No calibration was necessary to match the observed plume length.
Adsorption	• Retardation Factor: • Soil Bulk. Density pb: • foc: • Koc:	1.3 1.7 (kg/L) 0.08% B: 38 T: 135 E: 95 X: 240	• Calculated from R = 1+Koc x foc x pb/n • Estimated • Lab analysis • Literature - use Koc = 38
Biodegradation	Electron Acceptor: Background Conc. (mg/L): Minimum Conc. (mg/L): Change in Conc. (mg/L): Electron Acceptor: Max. Conc. (mg/L): Avg. Conc. (mg/L): Note: Boxed values are BIOSCREEN input values.	O2 NO3 SO4 6.0 17.0 100 - 0.22 - 0 - 0 [5.78] [17.0] [100] Fe: CH4 30.5 2.04 [11.3] [0.414]	• Based on July 1994 groundwater sampling program conducted by Parsons Engineering Science, Inc.
General	• Modeled Area Length: • Modeled Area Width: • Simulation Time:	1450 (ft) 320 (ft) 5 (yrs)	• Based on area of affected groundwater plume • Steady-state flow
Source Data	• Source Thickness: • Source Concentration:	10 (ft) (See Figure 5)	• Based on geologic logs and lumped BTEX monitoring data
Actual Data	Distance from Source (ft): BTEX Conc. (mg/L):	340 1080 1350 1420 8.0 1.0 0.02 0.005	• Based on observed concentration contour at site (see Figure 5)
OUTPUT	Centerline Concentration:	See Figure 7	
	Array Concentration:	See Figure 8	

Source Zone Assumption

Zone	Width (ft)	Source Conc. (mg/L)
3	100	9.0
2	25	2.8
1	50	0.07

Note: Source conc. based on geometric mean between concentration isopleth contours

Affected Soil Zone

Affected Groundwater Zone

Groundwater Flow Direction

SCALE (ft.)
0   200   400

Source of Data: Wiedemeier et al., 1995b.

LEGEND

⚴ Monitoring well location

▪ July 1994 Geoprobe sampling location

—8 0— BTEX concentration Isopleth, mg/L, July 1994

Affected Soil Zone

BIOSCREEN SOURCE ZONE ASSUMPTIONS

UST Site 870, Hill AFB, Utah

FIGURE 5

BIOSCREEN Modeling Summary Hill Air Force Base, UST Site 870, Utah:

- BIOSCREEN was used to try to reproduce the movement of the plume.

- An infinite source was assumed to simplify the modeling scenario. The source was assumed to be in the high concentration zone of the plume area (see Figure 5). Note that the zone of affected soil was quite large; however much of the affected soil zone downgradient of the source was relatively low concentration.

  Two modeling approaches could be applied: 1) assuming the source zone is just downgradient of the affected soil area (near well EPA-82-C) and ignoring the area upgradient of the this point, and 2) modeling most of the plume with source near MW-1. Alternative 1 is theoretically more accurate, as BIOSCREEN cannot account for the contributions from any affected soil zone downgradient of the source. At the case of Hill AFB, however, it was assumed that the contributions from this downgradient affected soil were relatively minor and that the main process of interest was the length of the plume from the high-concentration source zone. Therefore Alternative 2 was modeled, with the note that the middle of the actual plume may actually have higher concentrations than would be expected due to th contaminants in the downgradient affected soil zone.

- The instantaneous reaction model was used as the primary model to try to reproduce the plume length (~ 280 ft) as shown in Figure 7.

- The initial run of the instantaneous reaction model reproduced the existing plume without any need for calibration of dispersivity.

- As a check the first-order decay model was used with the BIOSCREEN default value of 2 yrs. This run greatly overestimated the plume length, so the amount of biodegradation was increased by decreasing the solute half-life. A half-life value of 0.1 years was required to match the plume length, although the match in the middle in the plume was much poorer.

- As shown in Figure 7, BIOSCREEN matches the observed plume fairly well. The instantaneous model is more accurate near the source while the first order decay model is more accurate near the middle of the plume. Both models reproduce the actual plume length relatively well.

- As shown in Figure 8, the model was unable to calculate the mass balances. A quick evaluation shows the reason: with a seepage velocity of 1600 ft/yr and a 5 year simulation time, the undegraded plume should be over 8000 ft long. Because the mass balance is based on a comparison of a complete undegraded plume vs. a degraded plume, a model area length of 8000 ft would be required for BIOSCREEN to complete the mass balance calculation. Therefore two runs would be needed to complete the simulation: 1) a run with a modeled length of 1450 feet to calibrate and evalute the match to existing data, and 2) a run with a modeled length of 8000 ft to do the mass balance. The results of the second run (change of model area length from 1450 ft to 8000 ft) indicate that over 99% of the mass that has left the source has biodegraded by the time groundwater has traveled 1450 ft.

Figure 6. BIOSCREEN Input Screen, Hill Air Force Base, Utah.

DISSOLVED HYDROCARBON CONCENTRATION ALONG PLUME CENTERLINE (mg/L at Z=0)

Distance from Source (ft.)

TYPE OF MODEL	0	145	290	435	580	725	870	1015	1160	1305	1450
No Degradation	9.000	8.?	7.465	6.684	6.089	5.624	5.250	4.940	4.679	4.455	4.260
1st Order Decay	9.000	4.348	1.969	0.905	0.424	0.201	0.096	0.047	0.023	0.011	0.005
Inst. Reaction	9.000	8.466	7.407	6.350	5.268	4.192	3.152	2.168	1.245	0.385	0.000
Field Data from Site	9.000		8.000					1.000		0.020	0.005

Time: 5 Years

Legend: 1st Order Decay · Instantaneous Reaction · No Degradation · Field Data from Site
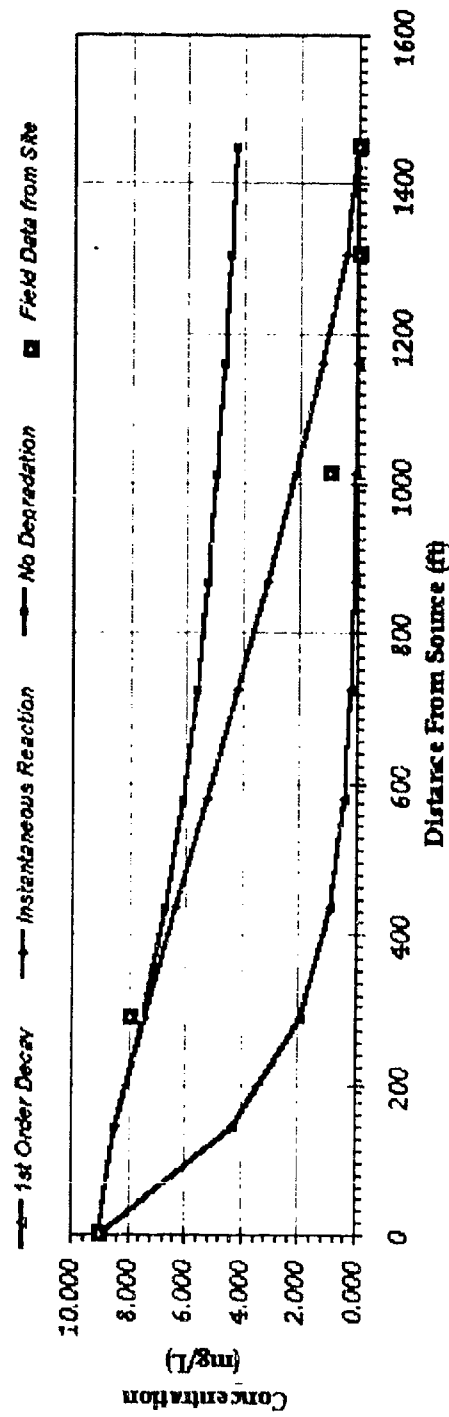
Concentration (mg/L) vs. Distance From Source (ft)

Figure 7. Centerline Output. Hill Air Force Base, Utah.

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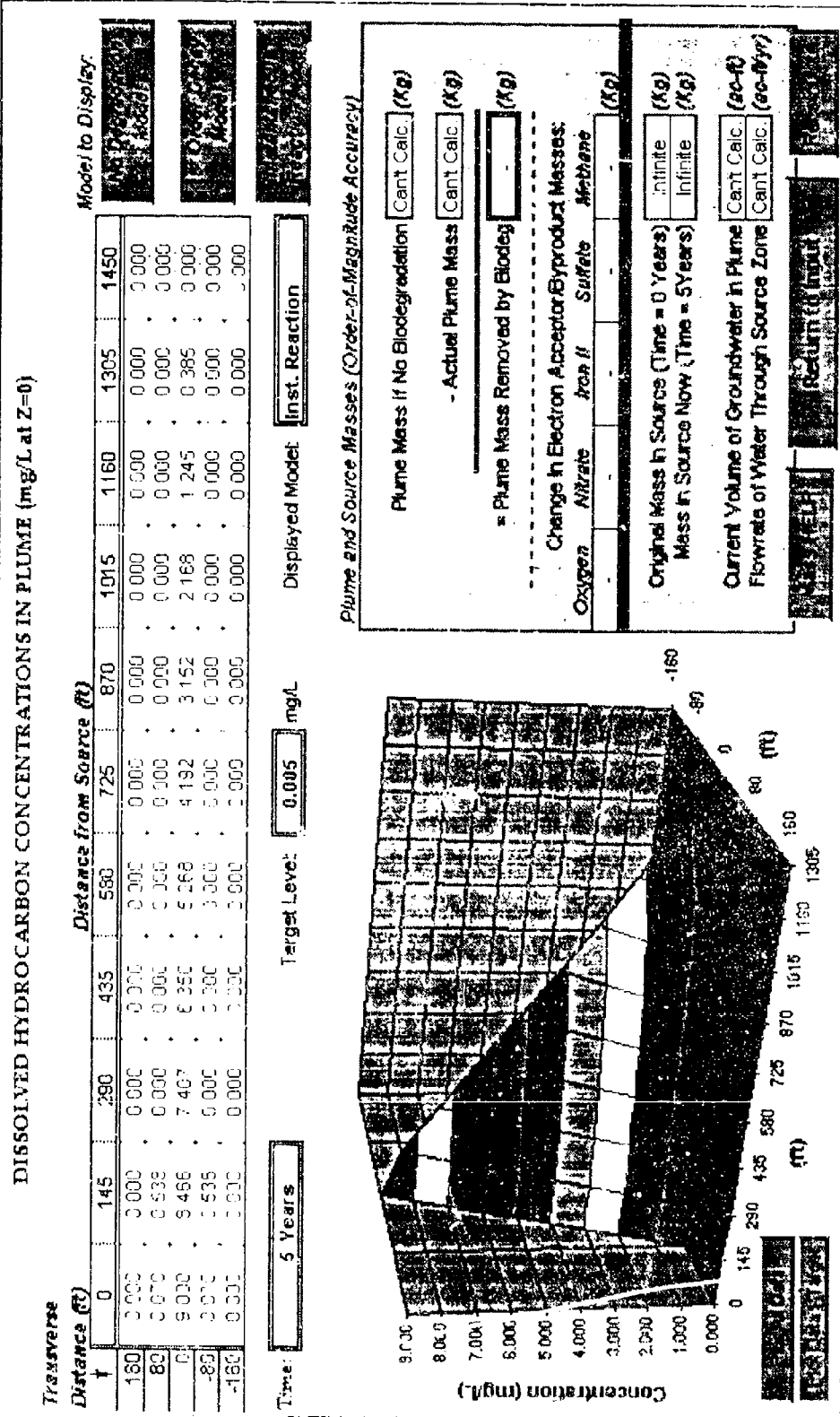
Figure 8. Array Concentration Output, Hill Air Force Base, Utah